Hooking Your Solver to AMPL

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ABSTRACT

This report tells how to make solvers work with AMPL's solve command. It describes an interface library, amplsolver.a, whose source is available from the AMPL web site in http://ampl.com/netlib/ampl (where updates first appear) and from *netlib*. Examples include programs for listing LPs, automatic conversion to the LP dual (shell-script as solver), solvers for various nonlinear problems (with first and sometimes second derivatives computed by automatic differentiation), and getting C or Fortran 77 for nonlinear constraints, objectives, and their first derivatives. Drivers for various well known linear, mixed-integer, and nonlinear solvers provide more examples.

CONTENTS

1. Introduction *Stub*.nl files

- Linear Problems
 Row-wise treatment
 Columnwise treatment
 Optional ASL components
 Example: *linrc*, a "solver" for row-wise printing
 Affine objectives: linear plus a constant
 Example: shell script as solver for the dual LP
- Integer and Nonlinear Problems
 Ordering of variables and constraints
 Reading nonlinear problems
 Evaluating nonlinear functions
 Example: nonlinear minimization subject to simple bounds
 Example: nonlinear least squares subject to simple bounds
 Partially separable structure
 Fortran variants
 Nonlinear test problems
- 4. Advanced Interface Topics Objective sense Accessing names Writing the *stub*.sol file Locating evaluation errors Imported functions Complementarity constraints

Suffixes Special Ordered Sets Checking for quadratic programs: example of a *DAG* walk C or Fortran 77 for a problem instance Writing *stub*.nl files for debugging Use with MATLAB or Octave

5. Utility Routines and Interface Conventions

-AMPL flag
Conveying solver options
Printing and Stderr
Formatting the optimal value and other numbers
A "Solver" for Gradients and Hessians: gjh
More examples
Evaluation Test Program
Multiple problems and multiple threads

1. Introduction

The AMPL modeling system [6,7] lets you express constrained optimization problems in an algebraic notation close to conventional mathematics. AMPL's solve command causes AMPL to instantiate the current problem, send it to a solver, and attempt to read a solution computed by the solver (for use in subsequent commands, e.g., to print values computed from the solution). This technical report tells how to arrange for your own solver to work with AMPL's solve command. See the AMPL web site (http://ampl.com) for much more information about AMPL.

Stub.nl files

AMPL runs solvers as separate programs and communicates with them by writing and reading files. The files have names of the form *stub*.*suffix*; AMPL usually chooses the *stub* automatically, but one can specify the *stub* explicitly with AMPL's write command. Before invoking a solver, AMPL normally writes a file named *stub*.nl. This file contains a description of the problem to be solved. AMPL invokes the solver with two arguments, the *stub* and a string whose first five characters are -AMPL, and expects the solver to write a file named *stub*.sol containing a termination message and the solution it has found.

Most linear programming solvers are prepared to read MPS files, which are described, e.g., in chapter 9 of [16]; see also the linear programming FAQ at

https://neos-guide.org/content/lp-faq

AMPL can be provoked to write an MPS file, *stub*.mps, rather than *stub*.nl, but MPS files are slower to read and write, entail loss of accuracy (because of rounding to fit numbers into 12-column fields), and can only describe linear and mixed-integer problems (with some differences in interpretations among solvers for the latter). AMPL's *stub*.nl files, on the other hand, contain a complete and unambiguous problem description of both linear and nonlinear problems, and they introduce no new rounding errors.

In the following, we assume you are familiar with C and that your solver is callable from C or C++. If your solver is written in some other language, it is probably callable from C, though the details are likely to be system-dependent. If your solver is written in Fortran 77, you can make the details system-independent by running your Fortran source through the Fortran-to-C converter f2c [5]; see http://ampl.com/netlib/f2c or http://www.netlib.org/f2c for more information, including source.

The AMPL/solver interface directory,

http://ampl.com/netlib/ampl/solvers

which is simply called solvers, in most of this document, contains some useful header files and source for a library, amplsolver.a, of routines for reading *stub*.nl and writing *stub*.sol files. Much of the rest of this report is about using routines in amplsolver.a. The entire solvers directory (without

subdirectories) is available as the gzipped tar file

http://ampl.com/netlib/ampl/solvers.tgz

A variant called solvers2, available as

http://ampl.com/netlib/ampl/solvers2.tgz

is useful with multiple threads, as explained at the end of this report. For large problems, nonlinear evaluations are often faster with solvers2 than with solvers, and the representations of nonlinearities take less memory, even with a single thread.

Material for many of the examples discussed here is in the solvers/examples directory, henceforth simply called "examples", available via such URLs as

```
http://ampl.com/netlib/ampl/solvers/examples
http://www.netlib.org/ampl/solvers/examples
```

or as the gzipped tar file http://ampl.com/netlib/ampl/solvers/examples.tgz. You will find it helpful to look at the files in examples while reading this report.

A "README" file in the solvers directory discusses compiling amplsolver.a, which on MS Windows systems is called amplsolv.lib. The instructions below for compiling examples assume you have already built amplsolver.a or amplsolv.lib, as appropriate.

2. Linear Problems

Row-wise treatment

For simplicity, we first consider linear programming (LP) problems. Solvers can view an LP as the problem of finding $x \in \mathbb{R}^n$ to

minimize or maximize
$$c^T x$$

subject to $b \le Ax \le d$ (LP)
and $\ell \le x \le u$

where $A \in \mathbb{R}^{m \times n}$, $b, d \in \mathbb{R}^m$, and $c, \ell, u \in \mathbb{R}^n$. The initial examples of reading linear problems just print out the data (A, b, c, d, ℓ, u) and perhaps the primal and dual initial guesses.

The first example, examples/lin1.c, just prints the data. The examples directory contains *makefile* variants makefile.u for Unix and Linux and makefile.vc for MS Windows. These *makefile* variants have rules for compiling and linking various examples. On a Unix or Linux system, initially give the command

```
cp makefile.u makefile
```

and under MS Windows, in a Commands window give the command

copy makefile.vc makefile

If necessary, you can then make changes to "makefile". For example, makefile.u and makefile.vc assume that solvers is the parent directory. If solvers is somewhere else, you should change the line

S = ..

suitably, replacing "..." with a relative or absolute path to your solvers or solvers2 directory. After this preparation, under Unix or Linux, invoke

make lin1

to compile and load the "lin1" program. Under MS Windows, the corresponding command would be

nmake lin1.exe

File lin1.c starts with

#include "asl.h"

i.e., asl.h from your solvers directory, as specified by the "S = ..." line in the makefile. The phrase "asl" or "ASL" that appears in many names stands for AMPL/Solver interface Library). In turn, asl.h includes various standard header files: math.h, stdio.h, string.h, stdlib.h, setjmp.h, and errno.h. Among other things, asl.h defines type ASL for a structure that holds various problem-specific data, and asl.h provides a long list of #defines to facilitate accessing items in an ASL when a pointer asl declared

ASL *asl;

is in scope. Among the components of an ASL are various pointers and such integers as the numbers of variables (n_var) , constraints (n_con) , and objectives (n_obj) . Most higher-level interface routines have their prototypes in asl.h, and a few more appear in getstub.h, which is discussed later. Also defined in asl.h are the types Long (usually the name of a 32-bit integer type, which is usually long or int), fint ('Fortran integer', normally a synonym for Long), real (normally a synonym for double), and ftnlen (also normally a synonym for Long, and used to convey string lengths to Fortran 77 routines that follow the f2c calling conventions).

The main routine in lin1.c expects to see one command-line argument: the *stub* of file *stub*.nl written by AMPL, as explained above. After checking that it has a command-line argument, the main routine allocates an ASL via

asl = ASL_alloc(ASL_read_f);

the argument to ASL_alloc determines how nonlinearities are handled and is discussed further below in the section headed "Reading nonlinear problems". The main routine appears to pass the *stub* to interface routine jacOdim, with prototype

```
FILE *jac0dim(char *stub, fint stub_len);
```

in reality, a #define in asl.h turns the call

```
jac0dim(stub, stublen)
```

into

```
jac0dim_ASL(asl, stub, stublen) .
```

There are analogous #defines in asl.h for most other high-level routines in amplsolver.a, but for simplicity, we henceforth just show the apparent prototypes (without leading asl arguments). This scheme makes code easier to read and preserves the usefulness of solver drivers written before the _ASL suffix was introduced.

For use with Fortran programs, jac0dim assumes stub is stublen characters long and does not assume stub is null-terminated. After trimming any trailing blanks from stub (by allocating space for ASL field filename, i.e., asl->i.filename_, and copying stub there as the *stub*), jac0dim reads the first part of *stub*.nl and records some numbers in *asl, as summarized in Table 1. If *stub*.nl does not exist, jac0dim by default prints an error message and stops execution (but setting return_nofile to a nonzero value changes this behavior: see Table 2 below).

To read the rest of *stub*.nl, lin1.c calls f_read. As discussed more fully below and shown in Table 6, several routines are available for reading *stub*.nl, one for each possible argument to ASL_alloc; f_read just reads linear problems, complaining and aborting execution if it sees any non-linearities. To acquire temporary memory — freed before f_read returns — f_read calls Malloc, which appears in most of our examples; Malloc calls malloc and aborts execution if malloc returns 0. To acquire memory that remains allocated when f_read returns, f_read calls Mlalloc, which uses Malloc and records the allocation, so all memory allocated by Mlalloc can be freed automatically when ASL_free(&asl) is called. The reason for breaking the reading of *stub*.nl into two steps will be seen in more detail below: sometimes it is convenient to modify the behavior of the *stub*.nl reader — here f_read — by allocating problem-dependent arrays before calling it.

AMPL may transmit several objectives. The linear part of each is contained in a list of ograd structures (declared in asl.h; note that asl.h declares

Component	Meaning	
n_var	number of variables (total)	
nbv	number of binary variables used linearly	
niv	number of other integer variables used linearly	
n_con	number of constraints (total)	
n_obj	number of objectives (total)	
nlo	number of nonlinear objectives: they come	
	before linear objectives	
nranges	number of ranged constraints:	
	$ \{i: -\infty < b_i < d_i < \infty\} $	
nlc	number of nonlinear general constraints,	
	including nonlinear network constraints	
nlnc	number of nonlinear network constraints:	
	they come after general nonlinear constraints	
*	and before any linear constraints	
nlvb	number of variables appearing nonlinearly	
*	in both constraints and objectives	
nlvbi	number of integer variables appearing nonlinearly	
	in both constraints and objectives	
nlvc	number of variables appearing nonlinearly in constraints	
nlvci	number of integer variables appearing nonlinearly	
	just in constraints	
nlvo *	number of variables appearing nonlinearly in objectives	
nlvoi	number of integer variables appearing nonlinearly	
	just in objectives	
lnc	number of linear network constraints	
nzc	number of nonzeros in the Jacobian matrix	
nzo	number of nonzeros in objective gradients	
maxrownamelen	length of longest constraint or	
	objective name (0 if no <i>stub</i> .row file)	
maxcolnamelen	length of longest variable name	
	(0 if no <i>stub</i> .col file)	
n_conjac[0]	Conval and Jacval operate on constraints <i>i</i> for	
n_conjac[1]	$n_{conjac[0]} \leq i < n_{conjac[1]},$	
	initially $n_{conjac}[0] = 0$ and	
	n_conjac[1] = n_con (all constraints)	
Table 1: ASL components set by jac0dim.		
* AMPL	versions \geq 19930630; otherwise nlvb = -1.	

- 5 -

typedef struct ograd ograd;

and has similar typedefs for all the other structures it declares). ASL field Ograd[i] points to the head of a linked-list of ograd structures for objective i + 1, so the sequence

allocates a scratch vector c, initializes it to zero, and (if there is at least one objective) stores the coefficients of the first objective in c. (The varno values in the ograd structure specify 0 for the first variable, 1 for the second, etc.)

Among the arrays allocated in lin1.c's call on f_read are an array of alternating lower and upper variable bounds called LUv and an array of alternating lower and upper constraint bounds called LUrhs. For the present exercise, these arrays could have been declared to be arrays of

struct LU_bounds { real lower, upper; };

however, for the convenience discussed below of being able to request separate lower and upper bound arrays, both LUv and LUrhs have type real*. Thus the code

```
printf("\nVariable\tlower bound\tupper bound\tcost\n");
for(i = 0; i < n_var; i++)
    printf("%8ld\t%-8g\t%-8g\t%g\n", i+1,
        LUv[2*i], LUv[2*i+1], c[i]);
```

prints the lower and upper bounds on each variable, along with its cost coefficient in the first objective.

For lin1.c, the linear part of each constraint is conveyed in the same way as the linear part of the objective, but by a list of cgrad structures. These structures have one more field,

int goff;

than ograd structures, to allow a "columnwise" representation of the Jacobian matrix in nonlinear problems; the computation of Jacobian elements proceeds "row-wise". The final for loops of lin1.c present the A of (LP) row by row. The outer loop compares the constraint lower and upper bounds against negInfinity and Infinity (declared in asl.h and available after ASL_alloc has been called) to see if they are $-\infty$ or $+\infty$.

Columnwise treatment

Most LP solvers expect a "columnwise" representation of the constraint matrix A of (LP). By allocating some arrays (and setting pointers to them in the ASL structure), you can make the *stub*.nl reader give you such a representation, with subscripts optionally adjusted for the convenience of Fortran. The next examples illustrate this. Their source files are lin2.c and lin3.c in examples, and you can say

make lin2 lin3

to compile and link them.

The beginning of lin2.c differs from that of lin1.c in that lin2.c executes

```
A_vals = (real *)Malloc(nzc*sizeof(real));
```

before invoking f_read. When a *stub.*nl reader finds A_vals non-null, it allocates integer arrays A_colstarts and A_rownos and stores the linear part of the constraints columnwise as follows: A_colstarts is an array of column offsets, and linear coefficient A_vals[*i*] appears in row A_rownos[*i*]; the *i* values for column *j* satisfy A_colstarts[*j*] $\leq i < A_colstarts[$ *j*+1] (in C notation). The column offsets and the row numbers start with the value Fortran (i.e., asl->i.Fortran_), which is 0 by default — the convenient value for use with C. For Fortran solvers, it is often convenient to set Fortran to 1 before invoking a *stub.*nl reader. This is illustrated in lin3.c, which also illustrates getting separate arrays of lower and upper bounds on the variables and constraints: if LUv and Uvx are not null, the *stub.*nl readers store the lower bound on the variables in LUv and the upper bounds in Uvx; similarly, if LUrhs and Urhsx are not null, the *stub.*nl readers store the area of null, the *stub.*nl readers store the lower bounds in LUrhs and the constraint upper bounds in Urhsx. Table 2 summarizes these and other ASL components that you can optionally set.

Optional ASL components

Table 2 lists some ASL (i.e., asl->i..._) components that you can optionally set and summarizes their effects.

Component	Туре	Meaning
return_nofile	int	If nonzero, jac0dim returns 0 rather than halting execution if <i>stub</i> .nl does not exist.
want_derivs	int	If you want to compute nonlinear functions but will never compute derivatives, reduce overhead by setting want_derivs = 0 (before calling the desired .nl reader). Alternatively, if you want nonlinear evaluations to succeed at points where first or second derivatives cannot be computed, set want_derivs = 2 (before calling the .nl reader).
Fortran	int	Adjustment to A_colstarts and A_rownos.
LUv	real*	Array of lower (and, if UVx is null, upper) bounds on variables.
Uvx	real*	Array of upper bounds on variables.
LUrhs	real*	Array of lower (and, if Urhsx is null, upper) constraint bounds.
Urhsx	real*	Array of upper bounds on constraints.
X0	real*	Primal initial guess: only retained if x0 is not null.
havex0	char*	If not null, $havex0[i] = 0$ means $X0[i]$ was specified (even if it is zero).
pi0	real*	Dual initial guess: only retained if pi0 is not null.
havepi0	char*	If not null, havepi0[i] != 0 means pi0[i] was specified (even if it is zero).
want_xpi0	int	<pre>want_xpi0 & 1 == 1 tells stub.nl readers to allocate X0 if a primal initial guess is available; want_xpi0 & 2 == 2 tells stub.nl readers to allocate pi0 if a dual initial guess is available; want_xpi0 & 4 == 4 tells stub.nl readers to allocate havex0 or havepi0 when reading X0 or pi0.</pre>
A_vals	real*	If not null, store linear Jacobian coefficients in A_vals, A_rownos, and A_colstarts rather than in lists of cgrad structures.
A_rownos	int*	Row numbers when A_vals is not null; allocated by <i>stub</i> .nl readers if necessary.
A_colstarts	int*	Column starts when A_vals is not null; allocated by <i>stub</i> .nl readers if necessary.
err_jmp	Jmp_buf*	If not null and an error occurs during nonlinear expression evaluation, longjmp here (without printing an error message).
err_jmp1	Jmp_buf*	If not null and an error occurs during nonlinear expression evaluation, longjmp here after printing an error message.
obj_no	fint	Objective number for writesol() and $qpcheck()$: 0 = first objective, $-1 = no$ objective, i.e., just find a feasible point.
	Table 2:	Optionally settable ASL components.

Example: *linrc*, a "solver" for row-wise printing

It is easy to extend the above examples to show the variable and constraint names used in an AMPL model. When writing *stub*.nl, AMPL optionally stores these names in files *stub*.col and *stub*.row, as described in §A18.4 (page 487–488) of the AMPL book [7]. As an illustration, example file linrc.c is a variant of linl.c that shows these names if they are available — and tells how to get them if they are not. Among other embellishments, linrc.c uses the value of environment variable display_width to decide when to break lines. (By the way, \$display_width denotes this value, and other environment-variable values are denoted analogously.) Say

make linrc

to create a linrc program based on linrc.c, and say

linrc '-?'

to see a summary of its usage. It can be used stand-alone, or as the "solver" in an AMPL session:

ampl: option solver linrc, linrc_auxfiles rc; solve;

will send a listing of the linear part of the current problem to the screen, and

ampl: solve >foo;

will send it to file foo. Thus linrc can act much like AMPL's expand and solexpand commands. See the AMPL book [7] (second edition) for more details on these commands.

Affine objectives: linear plus a constant

Adding a constant to a linear objective makes the problem no harder to solve. (The constant may be stated explicitly in the original model formulation, or may arise when AMPL's *presolve* phase deduces the values of some variables and removes them from the problem that the solver sees.) For algorithmic purposes, the solver can ignore the constant, but it should take the constant into account when reporting objective values. Some solvers, such as MINOS, make explicit provision for adding a constant to an otherwise linear objective. For other solvers, such as OSL and older versions of CPLEX[®], we must resort to introducing a new variable that is either fixed by its bounds (CPLEX) or by a new constraint (OSL). Function objconst, with apparent signature

real objconst(int objno)

returns the constant term for objective objno (with $0 \le objno < n_obj$) when that objective is linear. It returns 0 if objective objno is nonlinear. See the printing of the "Objective adjustment" in examples/linrc.c for an example of invoking objconst.

Example: shell script as solver for the dual LP

Sometimes it is convenient for the solver AMPL invokes to be a shell script that runs several programs, e.g., to transform *stub*.nl to the form the underlying solver expects and to create the *stub*.sol that AMPL expects. As an illustration, examples contains a shell script called dminos that arranges for minos to solve the dual of an LP. Why is this interesting? Well, sometimes the dual of an LP is much easier to solve than the original (''primal'') LP. Because of this, the CPLEX driver (http://ampl.com/netlib/solvers/cplex/cplex.c) has provision for solving the dual LP. (This is not to be confused with using the dual simplex algorithm, which might be applied to either the primal or the dual problem. The old OSL driver also had this provision.) Because minos is meant primarily for solving nonlinear problems (whose duals are more elaborate than the dual of an LP), minos currently lacks provision for solving dual LPs directly. At the cost of some extra overhead (over converting an LP to its dual within minos) and loss of flexibility (of deciding whether to solve the primal or the dual LP after looking at the problem), the dminos shell script provides an easy way to see how minos would behave on the dual of an LP. And one can use dminos to feed dual LPs to other LP solvers that understand *stub*.nl files: it's just a matter of setting the shell variable \$dsolver (which is discussed below).

The dminos shell script relies on a program called dualconv whose source, dualconv.c, also appears in examples. Dualconv reads the *stub*.nl for an LP and writes a *stub*.nl (or *stub*.mps) for the dual of the LP. Dualconv also writes a *stub*.duw file that it can use in a subsequent invocation to translate the *stub*.sol file from solving the dual LP into the primal *stub*.sol that AMPL expects. Thus dualconv is really two programs packaged, for convenience, as one. (Type

make dualconv to create dualconv and then

dualconv '-?'

for more detail on its invocation than we discuss below.)

Here is a simplified version of the dminos shell script (for Unix systems):

```
#!/bin/sh
dualconv $1
minos $1 -AMPL
dualconv -u $1
rm $1.duw
```

This simplified script and the fancier version shown below use Bourne shell syntax. In this syntax, \$1 is the script's first argument, which should be the *stub*. Thus

```
dualconv $1
```

passes the *stub* to dualconv, which overwrites *stub*.nl with a description of the dual LP (or complains, as discussed below). If all goes well,

```
minos $1 -AMPL
```

will cause minos to write stub.sol, and

dualconv -u \$1

will overwrite *stub*.sol with the form that AMPL expects. Finally,

rm \$1.duw

cleans up: in the usual case where AMPL chooses the *stub*, AMPL removes the intermediate files about which it knows (e.g., *stub*.nl and *stub*.sol), but AMPL does not know about *stub*.duw.

The simplified dminos script above does not clean up properly if it is interrupted, e.g., if you turn off your terminal while it is running. Here is the more robust examples/dminos:

```
#!/bin/sh
# Script that uses dualconv to feed a dual LP problem to $dsolver
dsolver=${dsolver-minos}
trap "rm -f $1.duw" 1 2 3 4 13
dualconv $1
case $? in 0)
        $dsolver $1 -AMPL
        case $? in 0) dualconv -u $1;; esac
        ;; esac
rc=$?
rm -f $1.duw
exit $rc
```

It starts by determining the name of the underlying solver to invoke:

```
dsolver=${dsolver-minos}
```

is an idiom of the Bourne shell that checks whether \$dsolver is null; if so, it sets \$dsolver to minos. The line

trap "rm -f \$1.duw" 1 2 3 4 13

arranges for automatic cleanup in the event of various signals. The next line

dualconv \$1

works as before. If all goes well, dualconv gives a zero exit code; but if dualconv cannot overwrite *stub*.nl with a description of the dual LP (e.g., because *stub*.nl does not represent an LP), dualconv complains and gives return code 1. The next line

case \$? in 0)

checks the return code; only if it is 0 is \$dsolver invoked. If the latter is happy (i.e., gives zero return code), the line

case \$? in 0) dualconv -u \$1;; esac

adjusts stub.sol appropriately. In any event,

rc=\$?

saves the current return code (i.e., \$? is the return code from the most recently executed program), since the following clean-up line

rm -f \$1.duw

will change \$?. Finally,

exit \$rc

uses the saved return code as dminos's return code. This is important, as AMPL only tries to read *stub*.sol if the solver gives a 0 return code.

To write *stub*.sol files, dualconv calls write_sol, which appears in most of the subsequent examples and is documented below in the section on "Writing the *stub*.sol file".

3. Integer and Nonlinear Problems

Ordering of integer variables and constraints

When writing *stub*.nl, AMPL orders the variables as shown in Tables 3 and 4 and the constraints as shown in Table 5. These tables also give expressions for how many entities are in each category. Table 4 applies to AMPL versions \geq 19930630; nlvb = -1 signifies earlier versions. For all versions, the first nlvc variables appear nonlinearly in at least one constraint. If nlvo > nlvc, the first nlvc variables may or may not appear nonlinearly in an objective, but the next nlvo - nlvc variables do appear nonlinearly in at least one objective. Otherwise all of the first nlvo variables appear nonlinearly in an objective. "Linear arcs" are linear variables declared with a noce declaration in the AMPL model, and "nonlinear network" constraints are nonlinear constraints introduced with a node declaration.

Category	Count	
nonlinear	max(nlvc, nlvo); see Table 4.	
linear arcs	nwv	
other linear	n_var - (max {nlvc, nlvo} + niv + nbv + nwv)	
linearly used binary	nbv	
linearly used other integer	niv	
Table 3: Ordering of Variables.		

Smoothness	Appearance	Count
continuous integer continuous integer	in an objective and in a constraint in an objective and in a constraint just in constraints just in constraints	nlvb - nlvbi nlvbi nlvc - (nlvb + nlvci) nlvci
continuous	just in objectives	max(0, nlvo – nlvc)
integer	just in objectives	nlvoi
	Table 4: Ordering of Nonlinea	ur Variables.

Category	Count	
nonlinear general	nlc-nlnc	
nonlinear network	nlnc	
linear network	lnc	
linear general	n_con-(nlc+lnc)	
Table 5: Ordering of Constraints.		

- 11 -

Reading nonlinear problems

It is convenient to build data structures for computing derivatives while reading a *stub*.nl file, and amplsolver.a provides several ways of doing this, to suit the needs of various solvers. Table 6 summarizes the available *stub*.nl readers and the kinds of nonlinear information they make available. They are to be used with ASL_alloc invocations of the form

asl = ASL_alloc(ASLtype);

Table 6's *ASLtype* column indicates the argument to supply for *ASLtype*. (This argument affects the size of the allocated ASL structure. Though we could easily arrange for a single routine to call the reader of the appropriate *ASLtype*, on some systems this would cause many otherwise unused routines from amplsolver.a to be linked with the solver. Explicitly calling the relevant reader avoids this problem.)

reader	ASLtype	nonlinear information		
f_read	ASL_read_f	no derivatives: linear objectives and constraints only		
fg_read	ASL_read_fg	first derivatives		
fgh_read [*]	ASL_read_fgh	first derivatives and Hessian-vector products		
pfg_read [*]	ASL_read_pfg	first derivatives and partially separable structure		
pfgh_read	ASL_read_pfgh	first and second derivatives and partially separable structure		
Table 6: stub.nl readers.				
* Not available in solvers2.				

All these readers have apparent signature

int reader(FILE *nl, int flags);

they close the nl file and return 0 if all goes well. The bits in the flags argument are described by comments in the enum ASL_reader_flag_bits declaration in asl.h; some of them pertain only to reading partially separable problems, which are discussed later, but others, such as ASL_return_read_err and ASL_rowwise_jac, are relevant to all the readers. The former governs the readers' behavior if they detect an error. If this bit is 0, the readers print an error message and abort execution; otherwise they return one of the nonzero values in enum ASL_reader_error_codes. See asl.h for details. Setting the ASL_rowwise_jac bit causes computed Jacobian matrices to be stored rowwise rather than columnwise.

Evaluating nonlinear functions

Specific evaluation routines are associated with each *stub*.nl reader. For simplicity, the readers supply pointers to the specific routines in the ASL structure, and asl.h provides macros to simplify calling the specific routines. The macros provide the following apparent signatures and functionality; many of them appear in the examples that follow. Reader pfg_read is mainly for debugging and does not provide any evaluation routines; it is used in solver "v8", discussed below. Reader fgh_read is mainly for debugging of Hessian-vector products, but does provide all of the routines described below except for the full Hessian computations (which would have to be done with n_var Hessian-vector products). Reader pfgh_read generally provides more efficient Hessian computations and provides the full complement of evaluation routines. If you invoke an "unavailable" routine, an error message is printed and execution is

aborted.

Many of the evaluation routines have final argument nerror of type fint*. This argument controls what happens if the routine detects an error. If nerror is null or points to a negative value, an error message is printed and, unless err_jmp1 (i.e., asl->i.err_jmp1_) is nonzero, execution is aborted. (You can set err_jmp1 much the same way that objlval_ASL and objlgrd_ASL in file objval.c set err_jmp to gain control after the error message is printed.) If nerror points to a nonnegative value, *nerror is set to 0 if no error occurs and to a positive value otherwise.

```
real objval(int nobj, real *X, fint *nerror)
```

returns the value of objective nobj (with $0 \le \text{nobj} < n_\text{obj}$) at the point X.

```
void objgrd(int nobj, real *X, real *G, fint *nerror)
```

computes the gradient of objective nobj and stores it in G[i], $0 \le i < n_var$.

void conval(real *X, real *R, fint *nerror)

evaluates the *bodies* of constraints at point X and stores them in R. Recall that AMPL puts constraints into the canonical form

left-hand side \leq *body* \leq *right-hand side*,

with left- and right-hand sides contained in the LUrhs and perhaps Urhsx arrays, as explained above in the section on "Row-wise treatment". Conval operates on constraints *i* with

 $n_{conjac[0]} \le i < n_{conjac[1]}$

(i.e., all constraints, unless you adjust the n_conjac values) and stores the body of constraint i in $R[i-n_conjac[0]]$, i.e., it stores the first constraint body it evaluates in R[0].

void jacval(real *X, real *J, fint *nerror)

computes the Jacobian matrix of the constraints evaluated by conval and stores it in J, at the goff offsets in the cgrad structures discussed above. In other words, there is one goff value for each nonzero in the Jacobian matrix, and the goff values determine where in J the nonzeros get stored. The *stub*.nl readers compute goff values so a Fortran program will see Jacobian matrices stored columnwise, but you can adjust the goff fields to make other arrangements.

```
real conival(int ncon, real *X, fint *nerror)
```

evaluates and returns the body of constraint ncon (with $0 \le n con < n_con$).

void congrd(int ncon, real *X, real *G, fint *nerror)

computes the gradient of constraint ncon and stores it in G. By default, congrd sets G[i], $0 \le i < n_var$, but if you set asl->i.congrd_mode = 1, it will just store the partials that are not identically 0 consecutively in G, and if you set asl->i.congrd_mode = 2, it will store them at the goff offsets of the cgrad structures for this constraint.

The following routines that compute Hessian-vector products or Hessians do not have an "X" argument and instead use partial derivatives computed in previous objective and constraint evaluations. It is the solver's responsibility to ensure that nonlinear constraints and objectives were most recently evaluated at the desired vector of primal variables.

```
void hvcomp(real *HV, real *P, int nobj, real *OW, real *Y)
```

stores in HV (a full vector of length n_var) the Hessian of the Lagrangian times vector P. In other words, hvcomp computes

$$\mathsf{HV} = W \cdot \mathsf{P},$$

where *W* is the Lagrangian Hessian,

$$W = \nabla^2 \left[\sum_{i=0}^{n_{obj}-1} \operatorname{OW}[i] f_i + \sigma \sum_{i=0}^{n_{obj}-1} \operatorname{Y}[i] c_i \right], \qquad (*)$$

DRAFT FOR COMMENT

in which f_i and c_i denote objective function *i* and constraint *i*, respectively, and σ is an extra scaling factor (most commonly +1 or -1) that is +1 unless specified otherwise by a previous call on lagscale (see below). If $0 \le \text{nobj} < \text{n_obj}$, hvcomp behaves as though OW were a vector of all zeros, except for OW[nobj], which is taken to be 1 if OW is null; otherwise, if OW is null, hvcomp behaves as though it were a vector of all zeros; and if Y is null, hvcomp behaves as though Y were a vector of zeros. *W* is evaluated at the point where the objective(s) and constraints were most recently computed (by calls on objval or objgrd, and on conval, conival, jacval, or congrd, in any convenient order). Normally one computes gradients before dealing with *W*, and if necessary, the gradient computing routines first recompute the objective(s) and constraints at the point specified in their argument lists. The Hessian computations use partial derivatives stored during the objective and constraint evaluations.

To make make it more efficient to call hvcomp(HV, P, nobj, OW, Y) several times at the same primal point with different P vectors but the same (nobj, OW, Y), some intermediate results may be saved from the first hvcomp call at the current point. In the unusual case of calling hvcomp(HV, P, nobj, OW, Y) at the same primal point but with a different value of the triple (nobj, OW, Y), it is necessary to first call $hvpinit(ihd_limit, nobj, OW, Y)$ with the new values of nobj, OW, and Y. This function has apparent signature

```
void hvpinit(int ihd lim, int nobj, real *OW, real *Y);
```

The first argument, ihd_lim, limits k in the size $k \times k$ of Hessians that are precomputed at new primal variable values; ihd_limit is #defined in asl.h to be asl->p.ihd_limit_, which by default is 12.

void duthes(real *H, int nobj, real *OW, real *Y)

evaluates and stores in H the dense upper triangle of the Hessian of the Lagrangian function W. Here and below, arguments nobj, OW and Y have the same meaning as in hvcomp, so duthes stores the upper triangle by columns in H, in the sequence

$$W_{0,0}$$
 $W_{0,1}$ $W_{1,1}$ $W_{0,2}$ $W_{1,2}$ $W_{2,2}$ · · ·

of length n var*(n var+1)/2 (with 0-based subscripts for W).

void fullhes(real *H, fint LH, int nobj, real *OW, real *Y)

computes the W of (*) and stores it in H as a Fortran 77 matrix declared

```
integer LH
double precision H(LH,*)
```

In C notation, fullhes sets

$$H[i + j \cdot LH] = W_{i,i}$$

for $0 \le i < n_var$ and $0 \le j < n_var$. Both duthes and fullhes compute the same numbers; fullhes first computes the Hessian's upper triangle, then copies it to the lower triangle, so the result is symmetric.

```
fint sphsetup(int nobj, int ow, int y, int uptri)
```

returns the number of nonzeros in the *sparse Hessian W* of the Lagrangian (*) (if uptri = 0) or its upper triangle (if uptri = 1) or its lower triangle (if uptri = 2), and stores in fields sputinfo->hrownos and sputinfo->hcolstarts a description of the sparsity of *W*, as discussed below with sphes. For sphes's computation, which determines the components of *W* that could be nonzero, arguments ow and y indicate whether OW and Y, respectively, will be zero or nonzero in subsequent calls on sphes. In analogy with hvcomp, duthes, fullhes and sphes, if $0 \le \text{nobj} < n_\text{obj}$, then nobj takes precedence over ow.

```
void sphes(real *H, int nobj, real *OW, real *Y)
```

computes the *W* given by (*) and stores it or its sparse upper triangle in H; sphsetup must have been called previously with arguments nobj, ow and y of the same sparsity (zero/nonzero structure), i.e., with the same nobj, with ow nonzero if ever OW will be nonzero, and with y nonzero if ever Y will be nonzero.

- 14 -

Argument uptri to sphsetup determines whether sphes computes W's upper triangle (uptri = 1) or all of W (uptri = 0); in the latter case, the computation proceeds by first computing the upper triangle, then copying it to the lower triangle, so the result is guaranteed to be symmetric. Fields sputinfo->hrownos and sputinfo->hcolstarts are pointers to arrays that describe the sparsity of W in the usual columnwise way:

$$H[j] = W_{i, rownows[j]}$$

for $0 \le i < n_var$ and hcolstarts $[i] \le j < hcolstarts[i+1]$. Before returning, sphsetup adds the ASL value Fortran to the values in the hrownos and hcolstarts arrays. The row numbers in hrownos for each column are in ascending order.

```
int xknown(real *X)
int xknowne(real *X, fint *nerror)
```

indicate that this X will be provided to the function and gradient computing routines in subsequent calls until either another xknown... invocation makes a new X known, or xunknown() is executed. The latter function, with apparent signature

void xunknown(void);

reinstates the default behavior of checking the X arguments against the previous value to see whether common expressions (or, for gradients, the corresponding functions) need to be recomputed. Appropriately calling xknown... and xunknown... can reduce the overhead in some computations. The nerror argument to xknowne() and xknowne_ew() is set to 0 if all goes well and to 1, 2, or 3 if a shared defined variable cannot be evaluated at this X. Values nerror = 2 or 3 are only possible when want_derivs was set to 2 (or another nonzero even value) before the *stub*.nl reader was called. The xknown() functions return 0 if the nonlinear components of X have not changed and 1 if they have changed since the last call on a routine in amplsolver.a that has an ''x'' argument.

```
void conscale(int i, real s, fint *nerror)
```

scales function body i by s, initial dual value pi0[i] by 1/s, and the lower and upper bounds on constraint i by s, interchanging these bounds if s < 0. This only affects the pi0, LUrhs and Urhsx arrays and the results computed by conval, jacval, conival, congrd, duthes, fullhes, sphes, and hvcomp. The write_sol routine described below takes calls on conscale into account.

```
void lagscale(real sigma, fint *nerror)
```

specifies the extra scaling factor $\sigma := sigma$ in the formula (*) for the Lagrangian Hessian.

void varscale(int i, real s, fint *nerror)

scales variable i, its initial value X0[i] and its lower and upper bounds by 1/s, and it interchanges these bounds if s < 0. Thus varscale effectively scales the partial derivative of variable i by s. This only affects the nonlinear evaluation routines and the arrays X0, LUv and Uvx. The write_sol routine described below accounts for calls on varscale.

Calls on conscale, varscale, and lagscale should be made after the $\mathit{stub.nl}$ reader has been called.

Example: nonlinear minimization subject to simple bounds

Our first nonlinear example ignores any constraints other than bounds on the variables and assumes there is one objective to be minimized. This example involves the PORT solver dmngb, which amounts to subroutine SUMSL of [8] with added logic for bounds on the variables (as described in [9]). Fortran source for PORT routines mentioned in this report, such as dmngb, is available in

 $\verb+http://ampl.com/netlib/ampl/solvers/examples/fport.zip+ and corresponding C source (via f2c) is available in+ for the source of the source$

http://ampl.com/netlib/ampl/solvers/examples/cport.zip The driver for this example is examples/mngl.c.

Most of mngl.c is specific to dmngb. For example, dmngb expects subroutine parameters calcf

and calcg for evaluating the objective function and its gradient. Interface routines objval and objgrd actually evaluate the objective and its gradient; the calcf and calcg defined in mngl.c simply adjust the calling sequences appropriately. The calling sequences for objval and objgrd were shown above.

- 15 -

Since dmngb is prepared to deal with evaluation errors (which it learns about when argument *NF to calcf and calcg is set to 0), calcf and calcg pass a pointer to 0 for nerror.

The main routine in mngl.c is called MAIN__ rather than main because it is meant to be used with an *f2c*-compatible Fortran library. (A C main appears in this Fortran library and arranges to catch certain signals and flush buffers. The main makes its arguments argc and argv available in the external cells xargc and xargv.)

Recall that when AMPL invokes a solver, it passes two arguments: the *stub* and an argument that starts with -AMPL. Thus mngl.c gets the *stub* from the first command-line argument. Before passing it to jac0dim, mngl.c calls ASL_alloc(ASL_read_fg) to make an ASL structure available. ASL_alloc stores its return value in the global cell cur_ASL. Since mngl.c starts with

#include "asl.h"
#define asl cur_ASL

the value returned by ASL_alloc is visible throughout mngl.c as "asl". This saves the hassle of making asl visible to calcf and calcg by some other means.

The invocation of dmngb directly accesses two ASL pointers: X0 and LUV (i.e., asl->i.X0_ and asl->i.LUV_). X0 contains the initial guess (if any) specified in the AMPL model, and LUV is an array of lower and upper bounds on the variables. Before calling fg_read to read the rest of *stub*.nl, mngl.c asks fg_read to save X0 (if an initial guess is provided in the AMPL model or data, and otherwise to initialize X0 to zeros) by executing

X0 = (real *)Malloc(n_var*sizeof(real));

After invoking dmngb, mngl.c writes a termination message into the scratch array buf and passes it, along with the computed solution, to interface routine write_sol, discussed later, which writes the termination message and solution to file *stub*.sol in the form that AMPL expects to read them.

The use of Cextern in the declaration

```
typedef void (*U_fp)(void);
Cextern int dmngb_(fint *n, real *d, real *x, real *b,
            U_fp calcf, U_fp calcg,
            fint *iv, fint *liv, fint *lv, real *v,
            fint *uiparm, real *urparm, U fp ufparm);
```

at the start of mngl.c permits compiling this example with either a C or a C++ compiler; Cextern is #defined in asl.h.

Example: nonlinear least squares subject to simple bounds

The previous example dealt only with a nonlinear objective and bounds on the variables. The next example deals only with nonlinear equality constraints and bounds on the variables. It minimizes an implicit objective: the sum of squares of the errors in the constraints. The underlying solver, dn2gb, again comes from the PORT subroutine library; it is a variant of the unconstrained nonlinear least-squares solver NL2SOL [3,4] that enforces simple bound constraints on the variables. Source for dn2gb appears in the files cport.zip and fport.zip mentioned above.

Source for this example is examples/nl21.c. Much like mng1.c, it starts with

#include "asl.h"
#define asl cur_ASL

followed by declarations for the definitions of two interface routines: calcr computes the residual vector (vector of errors in the equations), and calcj computes the corresponding Jacobian matrix (of first partial derivatives). Again these are just wrappers that invoke amplsolver.a routines described above,

conval and jacval. Parameter NF to calcr and calcj works the same way as in the calcf and calcg of mngl.c. Recall again that AMPL puts constraints into the canonical form

left-hand side \leq body \leq right-hand side.

Subroutine calcr calls conval to have a vector of n_con *body* values stored in array R. The MAIN__ routine in nl21.c makes sure the left- and right-hand sides are equal, and passes the vector LUrhs of left- and right-hand side pairs as parameter UR to dn2gb, which passes them unchanged as parameter UR to calcr. (Of course, calcr could also access LUrhs directly.) Thus the loop

in calcr converts the constraint body values into the vector of residuals.

MAIN__ invokes the interface routine dense_j() to tell jacval that it wants a dense Jacobian matrix, i.e., a full matrix with explicit zeros for partial derivatives that are always zero. If necessary, dense_j adjusts the goff components of the cgrad structures and tells jacval to zero its J array before computing derivatives.

Partially separable structure

Many optimization problems involve a partially separable objective function, one that has the form

$$f(x) = \sum_{i=1}^{q} f_i(U_i x),$$

in which U_i is an $m_i \times n$ matrix with a small number m_i of rows [13, 14]. Partially separable structure is of interest because it permits better Hessian approximations or more efficient Hessian computations. Many partially separable problems exhibit a more detailed structure, which the authors of LANCELOT [2] call "group partially separable structure":

$$f(x) = \sum_{i=1}^{q} \theta_i \left(\sum_{j=1}^{r_i} f_{ij}(U_{ij}x) \right),$$

where $\theta_i: \mathbb{R} \to \mathbb{R}$ is a unary operator. Using techniques described in [12], the *stub*.nl readers pfg_read and pfgh_read discern this latter structure automatically, and the Hessian computations that pfgh_read makes available exploit it. Some solvers, such as LANCELOT and VE08 [19], want to see partially separable structure. Driving such solvers involves a fair amount of solver-specific coding. Directory examples has drivers for two variants of VE08: ve08 ignores whereas v8 exploits partially separable structure, using reader pfg_read. Directory solvers/lancelot contains source for lancelot, a solver based on LANCELOT that uses reader pfgh_read.

Fortran variants

Fortran variants fmngl.f and fnl2l.f of mngl.c and nl2l.c appear in examples; the makefile has rules to make programs fmngl and fnl2l from them. Both invoke interface routines jacdim_ and jacinc_. The former allocates an ASL structure (with ASL_alloc(ASL_read_fg)) and reads a *stub*.nl file with fg_read, and the latter provides arrays of lower and upper constraint bounds, the initial guess, the Jacobian incidence matrix (which neither example uses), and (in the last variable passed to jacinc_) the value Infinity that represents ∞ . These routines have Fortran signatures

```
subroutine jacdim(stub, M, N, NO, NZ, MXROW, MXCOL)
character*(*) stub
integer M, N, NO, NZ, MXROW, MXCOL
subroutine jacinc(M, N, NZ, JP, JI, X, L, U, Lrhs, Urhs, Inf)
integer M, N, NZ, JP(N+1)
integer*2 JI
double precision X(N), L(N), U(N), Lrhs(M), Urhs(M), Inf
```

Jacdim_ sets its arguments as shown in Table 7. The values MXROW and MXCOL are unlikely to be of much interest; MXROW is 0 unless AMPL wrote *stub*.row (a file of constraint and objective names), in which case MXROW is the length of the longest name in *stub*.row. Similarly, MXCOL is 0 unless AMPL wrote *stub*.col, in which case MXROW is the length of the longest variable name in *stub*.col. Variant jacinc1() of jacinc() has argument JI of type fint* rather than short int*, i.e., of Fortran type integer rather than integer*2.

*M	= n_con	= number of constraints
*N	= n_var	= number of variables
*NO	= n_obj	= number of objectives
*NZ	= ncz	= number of Jacobian nonzeros
*MXROW	= maxrownamelen	= length of longest constraint name
*MXCOL	= maxcolnamelen	= length of longest variable name
	Table 7: Assignme	ents made by jacdim

The Fortran examples call Fortran variants of some of the nonlinear evaluation routines. Table 8 summarizes some Fortran variants; source and a test program for some others (e.g., for evaluating Hessian information) appear in

```
http://ampl.com/netlib/ampl/solvers/examples/fortmisc.zip
In Table 8, Fortran notation appears under "Fortran variant"; the corresponding C routines have an under-
score appended to their names and are declared in asl.h. The Fortran routines shown in Table 8 operate
on the ASL structure at which cur_ASL points. Thus, without help from a C routine to adjust cur_ASL,
they only deal with one problem at a time. After solving a problem and executing
```

call delprb

a Fortran code could call jacdim and jacinc again to start processing another problem.

Nonlinear test problems

Some nonlinear AMPL models appear in directory

http://ampl.com/netlib/ampl/models/nlmodels

The entire netlib/ampl/models directory, which has linear models, the nlmodels subdirectory, and directory compl for complementary problems, is available as the gzipped tar file

```
http://ampl.com/netlib/ampl/models.tgz
```

4. Advanced Interface Topics

Objective Sense

Whether objective n (0 $n < n_obj$) is to be minimized or maximized is specified by the objtype array: objtype[n] = 0 if it is to be minimized and objtype[n] = 1 if it is to be maximized.

Accessing names

Functions

```
char *con_name(int n);
char *obj_name(int n);
char *var_name(int n);
```

return the name of constraint $n \ (0 \le n < n_con)$, objective $n \ (0 \le n < n_obj)$, and variable $n \ (0 \le n < n_obj)$, respectively. If the relevant auxfiles option was suitably set when the stub.nl file was written, the names will be from the AMPL model. Otherwise they will be generic names, such as $_scon[1]$.

```
Routine
             Fortran variant
congrd
             congrd(N, I, X, G, NERROR)
conival
             cnival(N, I, X, NERROR)
conval
             conval(M, N, X, R, NERROR)
dense_j
             densej()
hvcomp
             hvcomp(HV, P, NOBJ, OW, Y)
jacval
             jacval(M, N, NZ, X, J, NERROR)
objgrd
             objgrd(N, X, NOBJ, G, NERROR)
objval
             objval(N, X, NOBJ, NERROR)
writesol
             wrtsol(MSG, NLINES, X, Y)
xknown
             xknown(X)
xunkno
             xunkno()
delprb_
             delprb()
                                    Description
Argument
             Type
Ν
             integer
                                    number of variables (n_var)
М
             integer
                                    number of constraints (n_con)
                                    number of Jacobian nonzeros (nzc)
ΝZ
             integer
NERROR
             integer
                                    if \geq 0, set NERROR to 0 if all goes well
                                    and to a positive value if the evaluation fails
Ι
             integer
                                    which constraint
                                    which objective
NOBJ
             integer
NLINES
             integer
                                    lines in MSG
                                    solution message, dimension(NLINES)
MSG
             character*(*)
Χ
             double precision
                                    incoming vector of variables
G
             double precision
                                    result gradient vector
             double precision
                                    result Jacobian matrix
J
OW
             double precision
                                    objective weights
             double precision
Υ
                                    dual variables
Ρ
             double precision
                                    vector to be multiplied by Hessian
НV
             double precision
                                    result of Hessian times P

        Table 8: Fortran variants.
```

- 18 -

Writing the *stub*.sol file

Interface routine write_sol returns the computed solution and a termination message to AMPL by writing a *stub*.sol file. (When the solver is not invoked by AMPL, the .sol file is only written if "-AMPL" was given as the second command-line argument or the wantsol keyword has an odd value.) This routine has apparent prototype

void write_sol(char *msg, real *x, real *y, Option_Info *oi);

The first argument is for the (null-terminated) termination message. It should not contain any empty embedded lines (though, e.g., " \n ", i.e., a line consisting of a single blank, is fine) and may end with an arbitrary number of newline characters (including none, as in mngl.c). The second and third arguments, x and y, are pointers to arrays of primal and dual variable values to be passed back to AMPL. Either or both may be null (as is y in mngl.c), which causes no corresponding values to be passed. Normally it is helpful to return the best approximate solution found, but for some errors (such as trouble detected before the solution algorithm can be started) it may be appropriate for both x and y to be null. The fourth argument points to an optional Option_Info structure, which is discussed below in the section on "Conveying solver options". Before calling write_sol(), a solver should assign a suitable value to solve_result_num (i.e., asl->i.solve_result_num_); see pp. 283–284 of [7].

- 19 -

Locating evaluation errors

If the routines in amplsolver.a detect an error during evaluation of a nonlinear expression, they look to see if *stub*.row (or, if evaluation of a "defined variable" was in progress, *stub*.fix) is available. If so, they use it to report the name of the constraint, objective, or defined variable that they were trying to evaluate. Otherwise they simply report the number of the constraint, objective, or variable in question (first one = 1). This is why AMPL provides the default value RF for \$minos_auxfiles. See the discussion of auxiliary files in §A18.4 of the AMPL book [7]; as documented in *netlib*'s "changes from ampl", i.e.,

http://ampl.com/netlib/ampl/changes

capital letters in *\$solver_auxfiles* have the same effect as their lower-case equivalents on nonlinear problems, including problems with integer variables, and have no effect on purely linear problems.

Imported functions

An AMPL model may involve imported functions. If invocations of such functions involve variables, the solver must be able to evaluate the functions. You can tell your solver about the relevant functions by supplying a suitable funcadd function, rather than loading a dummy funcadd compiled from solvers/funcadd0.c. Include file funcadd.h gives funcadd's prototype:

void funcadd(AmplExports *ae);

Among the fields in the AmplExports structure are some function pointers, such as

also in funcadd.h are #defines that simplify using the function pointers, assuming

AmplExports *ae

is visible. In particular, funcadd.h gives addfunc the apparent prototype

To make imported functions known, funcadd should call addfunc once for each one. The first argument, name, is the function's name in the AMPL model. The second argument points to the function itself. The type argument tells whether the function is prepared to accept symbolic arguments (character strings): 0 means "no", 1 means "yes". Argument nargs tells how many arguments the function expects; if nargs ≥ 0 , the function expects exactly that many arguments; otherwise it expects at least -(nargs + 1). (Thus nargs = -1 means 0 or more arguments, nargs = -2 means 1 or more, etc. The argument counting and type checking occur when the *stub*.nl file is subsequently read.) Finally, argument funcinfo is for the function to use as it sees fit; it will subsequently be passed to the function in field funcinfo of struct arglist.

When an imported function is invoked, it always has a single argument, al, which points to an arglist structure. This structure is designed so the same imported function can be linked with AMPL (in case AMPL needs to evaluate the function); the final arglist components are relevant only to AMPL. The function receives al->n arguments, al->nr of which are numeric; for $0 \le i < al->n$,

if $al \rightarrow at[i] \ge 0$, argument *i* is $al \rightarrow ra[al \rightarrow at[i]]$ if $al \rightarrow at[i] < 0$, argument *i* is $al \rightarrow sa[-(al \rightarrow at[i] + 1)]$.

If al->derivs is nonzero, the function must store its first partial derivative with respect to al->ra[*i*] in al->derivs[*i*], and if al->hes is nonzero (which is possible only with fgh_read or pfgh_read), it must also store the upper triangle of its Hessian matrix in al->hes, i.e., for

 $0 \le i \le j < al ->nr$

it must store its second partial with respect to al - ra[i] and al - ra[j] in

 $al \rightarrow hes[i + \frac{1}{2}j(j+1)]$. Sometimes partials with respect to some arguments are not needed, in which case $al \rightarrow dig$ is nonzero, and $al \rightarrow dig[i]$ is nonzero if partials with respect to

al->ra[i] will not be used. It is always safe to provide all partials.

If the function does any printing, it should initially say

AmplExports *ae = al->AE;

to make special variants of printf available.

See solvers/funcadd.c for an example funcadd. The mng, mnh and nl2 examples mentioned below illustrate linking with this funcadd.

When an imported function is called by AMPL, ae->asl is null and calls on getenv(name), which is #defined to be (*ae->Getenv)(name), return values affected by AMPL's option commands. When an imported function is called by a solver, ae->asl is the solvers's ASL pointer.

If an imported function cannot perform as expected, it should set al->Errmsg to a string explaining the trouble. If the function returns a function value but cannot compute first derivatives, acl->Errmsg should start with a single single quote ('); if the function returns a function value and first derivatives but cannot compute second derivatives, al->Errmsg should start with a double-quote character ("). If need be, memory *n* bytes long to hold this string can be allocated by calling ae->Tempmem(al->TMI, n), which returns a void* value. The ae->Tempmem() function can also be called to obtain memory for any other use during the current invocation of an imported function. Such memory is automatically freed after the function returns — and after use is made of al->Errmsg.

Complementarity Constraints

Constraints involving complementarity conditions are declared with the complements keyword in an AMPL model, which causes the *stub*.nl readers to allocate and populate a cvar array that indicates which constraints are involved in complementarity conditions. Suppose cvar[i] = j. If j = 0, then constraint *i* is an ordinary algebraic constraint, but if j > 0, then the constraint complements variable j-1. In this latter case, if the constraint has one finite bound, then the variable will also have one finite bound, and either the constraint or the variable must be at its bound. If the constraint has distinct finite lower and upper bounds, then the variable has no explicit bounds, but must be nonnegative if the constraint is at its lower bound, nonpositive if the constraint is at its upper bound, and zero if the constraint is strictly slack.

Some solvers are not prepared to handle general complementarity conditions, but do handle conditions of the form $v_i \ge 0$, $v_j \ge 0$, $min(v_i, v_j) = 0$. Such solvers should set the ASL_cc_simplify bit in the flags argument to the *stub*.nl reader, which causes the reader to allocate arrays asl->i.ccindl and asl->i.ccind2 and to adjust the problem so there are n_cc complementarity conditions of the form

variable asl->ccind1[*i*] ≥ 0 *variable* asl->ccind2[*i*] ≥ 0

and

min(variable asl->ccind1[i], variable asl->ccind2[i]) = 0.

Suffixes

AMPL models can declare suffixes, which are names for auxiliary values associated with variables, constraints, objectives, and problems. Some of these values may be inputs to the solver, others may be values computed by the solver and returned to the AMPL session, and some may be both. For example, some solvers allow one to specify an incoming basis and to return a final basis; basic variables and constraints are conventionally indicated by .sstatus suffixes on variables and constraints. AMPL can send initial .sstatus values to the solver and retrieve updated .sstatus values from the .sol file that the solver writes. Some suffixes assume only a small number of integer values or ranges of such values, and sometimes it is convenient to have symbolic descriptions of these (ranges of) values. For example, when AMPL begins execution, option sstatus_table has the value

0 none no status assigned

```
bas
            basic\
1
2
   sup
            superbasic\
3
            nonbasic <= (normally =) lower bound\</pre>
    low
4
            nonbasic >= (normally =) upper bound\
  upp
            nonbasic at equal lower and upper bounds\
5
    equ
            nonbasic between bounds
6
    btw
```

For suffixes that have an associated "_table" option value (which one can supply and modify as desired), AMPL uses the value in the second column of the table as the displayed value of the suffix when its numeric value is at most the value in the first column (and exceeds the first-column value of the previous row, if any, of the table); one can print or display the suffix's numeric value by appending "_num" to the suffix's name. When changing a suffix's value in a "let" command, one can use either a numeric or string for the new value. For example:

```
ampl: display x.sstatus, x.sstatus_num;
x.sstatus = none
x.sstatus_num = 0
ampl: let x.sstatus := 3;
ampl: display x.sstatus, x.sstatus_num;
x.sstatus = low
x.sstatus_num = 3
ampl: let x.sstatus := 'upp';
ampl: display x.sstatus, x.sstatus_num;
x.sstatus = upp
x.sstatus_num = 4
```

Before accessing incoming status values or supplying outgoing status values, a solvers must invoke

```
suf_declare(suftab, nsuftab);
```

in which suftab is an array of SufDecl structures:

```
struct SufDecl {
    /* Pass array of SufDecl's to suf_declare(). */
    char *name;
    char *table;
    int kind;
    int nextra;
    };
```

and nsuftab is the number of SufDecl values in the suftab array. Usually the table value is null, but it can be the value desired for the suffix's _table option when the suffix is returned to the AMPL session. The kind value should be one of

```
ASL_Sufkind_var = 0,
ASL_Sufkind_con = 1,
ASL_Sufkind_obj = 2,
ASL_Sufkind_prob = 3,
```

to indicate a suffix on variables, constraints, objectives, or problems, respectively, possibly or-ed with one or more of

```
ASL_Sufkind_real = 4, /* use SufDesc.u.r rather than .i */
ASL_Sufkind_iodcl = 8, /* declare as INOUT suffix */
ASL_Sufkind_output = 16, /* return this suffix to AMPL */
ASL_Sufkind_input = 32, /* input values were received from AMPL */
ASL_Sufkind_outonly = 64 /* reject as an input value */
```

The *stub*.nl reader sets the ASL_Sufkind_input bit for suffixes retrieved from the incoming *stub*.nl file.

Suffixes are stored in integer arrays unless ASL_Sufkind_real is specified. Suffixes like sstatus that can appear on more than one kind of entity must have a separate SufDecl entry for each kind. For example, the CPLEX driver http://ampl.com/netlib/ampl/solvers/cplex.chas a suftab declaration with many SufDecl values, including

- 22 -

```
{ "iis", iis_table, ASL_Sufkind_var | ASL_Sufkind_outonly },
{ "iis", 0, ASL_Sufkind_con | ASL_Sufkind_outonly },
{ "lazy", 0, ASL_Sufkind_con },
...
{ "sstatus", 0, ASL_Sufkind_var, 1 },
{ "sstatus", 0, ASL_Sufkind_con, 1 },
```

Thus .iis can be a suffix on both constraints and variables. This suffix is for describing an "irreducible infeasible" set of mutually inconsistent constraints and variables. The iis_table permits using symbolic names for the suffix values. It is only necessary to supply iis_table once. Its declaration is

```
static char iis table[] = "n
       not in the iis\n\
0
   non
1
          at lower bound\n\
   low
2
   fix
         fixed\n\
3
   upp
         at upper bound\n\
4
         member\n\
   mem
5
   pmem possible member\n\
        possibly at lower bound\n\
6
  plow
7
           possibly at upper boundn
   pupp
8
   bug\n";
```

To access incoming suffix values, one invokes suf_get() with apparent prototype

SufDesc *suf_get(const char *sufname, int kind);

For example, to see if there is an incoming .lazy suffix (as declared in the partial suftab declaration shown above), one would use coding of the form

```
SufDesc *lazy;
...
lazy = suf_get("lazy", ASL_Sufkind_con);
```

If the resulting lazy->u.i value is null, then the .lazy suffix is not available. Otherwise lazy->u.i is an arrary (of integers) giving the .lazy suffix values on constraints. If ASL_Sufkind_real had been specified for this suffix, then lazy->u.r would be the (possibly null) array of 'real' values for the suffix. By or-ing ASL_Sufkind_input onto the kind argument to suf_get, e.g.,

lazy = suf_get("lazy", ASL_Sufkind_con | ASL_Sufkind_input);

one can request that null be returned for lazy if incoming .lazy values are not present in the *stub*.nl file.

To return suffix values to AMPL for a suffix not declared with ASL_Sufkind_output in its suftab entry, one invokes apparent prototype

SufDesc *suf_iput(const char *sufname, int kind, int *val);

for an integer-valued suffix or

SufDesc *suf_rput(const char *sufname, int kind, real *val);

for a "real" valued one. The val argument should be the arrary that will contain the desired outgoing suffix values. The value returned by suf_iput or suf_rput is that which suf_get(...) would have returned.

Special Ordered Sets

Special ordered sets [1] are useful for expressing situations where one of several alternatives must be chosen (type 1 SOS sets) and general piecewise-linear functions (type 2). An SOS set of type 1 is a set of binary variables, exactly one of which can be 1, conveniently expressed as $\sum b_i = 1$, and an SOS set of

type 2 is an ordered set of binary variables such that at most two are nonzero, and two nonzero such variables are adjacent. A convex piecewise-linear function, when appearing in an objective to be minimized or on the left-hand side of a \geq constraint, can be expressed by several linear inequality contraints, but a more general piecewise-linear function appearing in such places needs to involve an SOS set of type 2. AMPL uses SOS sets of type 2 to "linearize" nonconvex piecewise-linear functions, so they can be treated by a mixed-integer linear programming solver. The resulting *stub*.nl file will work with any such solver, but solvers that are prepared to handle SOS sets explicitly may work more efficiently when told about SOS sets. To facilitate this, AMPL attaches suffixes .sosno and .sosref to relevant variables. In AMPL declarations and scripts, one can also supply suffixes .sosno and .ref to manually express SOS sets. Each has a distinct .sosno value, with positive values for SOS type 1 sets and negative values for type 2 sets. Solvers can call suf_sos(), with apparent signature

to obtain SOS details in the arrays allocated by suf_sos() and to remove relevant constraints supplied by AMPL for conveying nonconvex piecewise-linear terms. This function returns the number of SOS sets so treated. The flags argument determines which SOS sets are treated. It is an "or" of

ASL_suf_sos_explict_free ASL_suf_sos_ignore_sosno ASL_suf_sos_ignore_amplso

(declared in asl.h). ASL_suf_sos_explict_free means the caller will explicitly free arrays allocated by suf_sos(); otherwise the arrays will be freed automatically when ASL_free(&asl) is called. ASL_suf_sos_ignore_sosno causes suf_sos() to ignore any .sosno and .ref suffixes, and ASL_suf_sos_ignore_amplso causes suf_sos() to ignore the .sos and .sosref suffixes AMPL uses for nonconvex piecewise-linear terms. After the call

the arrays allocated by $suf_sos()$ describe nsos SOS sets. A total of nsosnz variables are involved in these sets. For $0 \le i < nsos$, set *i* is of type sostype[i] and has variables sosind[j] with weight sosref[j] for $sosbeg[i] \le j < sosbeg[i + 1]$.

Solver drivers that use suf_sos() include cplex/cplex.c, gurobi/gurobi.c, and xpress/xpress.c in http://ampl.com/netlib/ampl/solvers.

Checking for quadratic programs: example of a DAG walk

Some solvers make special provision for handling quadratic programming problems, which have the form

minimize or maximize
$$\frac{1}{2}x^{T}Qx + c^{T}x$$

subject to $b \le Ax \le d$ (QP)
and $\ell \le x \le u$

in which $Q \in \mathbb{R}^{n \times n}$. Various solvers handle general positive-definite Q matrices, and the old KORBX solver handled positive-definite diagonal Q matrices ("convex separable quadratic programs"). These solvers generally assume the explicit $\frac{1}{2}$ shown above in the (QP) objective.

AMPL considers quadratic forms, such as the objective in (QP), to be nonlinear expressions. To determine whether a given objective function is a quadratic form, it is necessary to walk the directed acyclic graph (DAG) that represents the (possibly) nonlinear part of the objective. For just determining whether an

objective or a constraint is quadratic, function degree with apparent signature

does a simple graph walk on objective co if $0 \le co < n_obj$ or on constraint -(co+1) if $0 \le -(co+1) < n_con$ and returns

$$-1 = bad co value$$

 $0 = constant$
 $1 = linear$
 $2 = quadratic$
 $3 = general nonlinear.$

The pv argument should be null if degree(...) is to be called just once (e.g., to see if the objective is quadratic). If multiple calls are expected (e.g., for objectives and constraints), it may save time to use the pattern

```
void *v = 0;
for(...) { ... degree(asl, co, &v); ... }
if (v) free(v);
```

Function degree and the qpcheck variants discussed next are meant to be used with a variant of fg_read called qp_read that has the same prototype as the other *stub*.nl readers, and which changes some function pointers to integers for the convenience of the qpcheck functions. After qp_read returns, you can invoke degree or nqpcheck, etc., one or more times, but you may not call objval, conval, etc., until you have called qp_opify, with apparent prototype

void qp_opify(void)

to restore the function pointers. With solvers2, one can simply call the desired *stub*.nl reader rather than qp_read(), and there is no need to call qp_opify(), which does nothing when solvers2 is used.

Function nqpcheck (in solvers/nqpcheck.c) illustrates a more detailed graph walk that can determine quadratic coefficients. This function has apparent prototype

```
fint nqpcheck(int co, fint **rowqp, fint **colqp, real **delsqp);
```

its first argument indicates the constraint or objective to which it applies: $co \ge 0$ means objective co, and co < 0 means constraint -(co + 1). If the relevant objective or constraint is a quadratic form with Hessian Q, nqpcheck returns the number of nonzeros in Q (which is 0 if the function is linear), and sets its pointer arguments to pointers to arrays that describe Q. Specifically, *delsqp points to an array of the nonzeros in Q, *rowqp to their row numbers (first row = Fortran), and *colqp to an array of subscripts, incremented by Fortran, of the first entry in *rowqp and *delsqp for each column, with (*colqp)[n_var] giving the subscript just after the last column. Nqpcheck sorts the nonzeros in each column of Q by their row indices and returns a symmetric Q. For non-quadratic functions, npqcheck returns -1; it returns -2 in the unlikely case that it sees a division by 0, and -3 if co is out of range.

For solvers that only deal with one objective, it may be more convenient to call qpcheck rather than nqpcheck; qpcheck has apparent prototype

fint qpcheck(fint **rowqp, fint **colqp, real **delsqp);

It looks at objective obj_no (i.e., asl->i.obj_no_, with default value 0) and complains and aborts execution if it sees something other than a linear or quadratic form. When it sees one of the latter, it gives the same return value as nqpcheck and sets its arguments the same way.

Arguments rowqp, colqp, and delsqp to nqpcheck() and qpcheck() can be null; the return value is unaffected. When these arguments are not null, the memory pointed to by *rowqp, *colqp, and *delsqp is automatically freed when ASL_free(&asl) is called. Variant

fint mqpcheck(int co, fint **rowqp, fint **colqp, real **delsqp);

of nqpcheck() assigns values to *rowqp, *colqp, and *delsqp that are allocated individually by malloc() and must be freed by explicit calls on free().

Some solvers have specific ways of handling quadratic constraints. Such solvers can avoid some overhead by calling

ssize_t mqpcheckv(int co, QPinfo **QPIp, void **vp);

once per constraint (or objective), with final argument &v and with v initialized to null before the first call. Some auxiliary arrays are constructed and stored in memory pointed to by v and are reused on subsequent calls on mqpcheckv(). After the final such call, one invokes mqpcheckv_free(&v) to dispose of the auxiliary arrays; v is set to null by this call. (In calls on mqpcheckv(), the vp argument can itself be null, in which case the the auxiliary arrays are constructed anew on each call and are freed before mqpcheckv() returns.)

The QPIp argument to mqpcheckv() can be null. When it is not null, it is set to point to a QPinfo structure declared in asl.h:

```
typedef struct QPinfo {
```

On most systems that use 64-bit addressing, size_t is an unsigned 64-bit integer, which allows addressing more than 2³¹ nonzeros, and ssize_t is a signed variant of size_t. (Though size_t is a standard type, on some systems it may be necessary to provide a suitable #define or typedef for ssize_t.) The QPI value returned by mqpcheckv(co, &QPI, vp), and the arrays whose values QPI contains are all allocated by a single malloc() call, so when done with QPI, a solver should call free(QPI) to dispose of QPI and the arrays to which it points.

Before returning quadratic details, the qpcheck() variants adjust constraint bounds and the objconst() function to account for constant terms.

Drivers cplex.c, gurobi/gurobi.c, and xpress/xpress.c call qp_read and qpcheck, and file examples/qtest.c illustrates invocations of nqpcheck and qp_opify.

More elaborate *DAG* walks are useful in other situations. For example, the nlc program discussed next does a more detailed *DAG* walk.

C or Fortran 77 for a problem instance: *nlc*

Occasionally it may be convenient to turn a *stub*.nl file into C or Fortran. This can lead to faster function and gradient computations — but, because of the added compile and link times, many evaluations are usually necessary before any net time is saved. Program nlc converts *stub*.nl into C or Fortran code for evaluating objectives, constraints, and their derivatives. You can get source for nlc as

http://ampl.com/netlib/ampl/solvers/nlc.tgz

By default, nlc emits C source for functions feval_ and ceval_; the former evaluates objectives and their gradients, the latter constraints and their Jacobian matrices (first derivatives). These functions have signatures

real feval_(fint *nobj, fint *needfg, real *x, real *g); void ceval_(fint *needfg, real *x, real *c, real *J);

For both, x is the point at which evaluations take place, and *needfg tells whether the routines compute function values (if *needfg = 1), gradients (if *needfg = 2), or both (if *needfg = 3). For feval_,

*nobj is the objective number (0 for the first objective), and g points to storage for the gradient (when *needfg = 2 or 3). For ceval_, c points to storage for the values of the constraint bodies, and J points to columnwise storage for the nonzeros in the Jacobian matrix. Auxiliary arrays

```
extern fint funcom_[];
extern real boundc_[], x0comn_[];
extern fint auxcom_[1];
```

describe the problem dimensions, nonzeros in the Jacobian matrix, left- and right-hand sides of the constraints, bounds on the variables, the starting guess, and the number of nonlinear constraints (which come first). Specifically,

> funcom_[0] = n_var = number of variables; funcom_[1] = n_obj = number of objectives; funcom_[2] = n_con = number of constraints; funcom_[3] = nzc = number of Jacobian nonzeros; funcom [4] = densej is zero in the default case that the Jacobian matrix is stored

sparsely, and is 1 if the full Jacobian matrix is stored (if requested by the -d command-line option to nlc).

funcom_[i], $5 \le i \le 4 + n_{obj}$, is 1 if the objective is to be maximized and 0 if it is to be minimized. If densej = funcom_[4] is 0, then colstarts = funcom_ + n_obj + 5 and rownos = funcom_ + n_obj + n_var + 6 are arrays describing the nonzeros in the columns of the Jacobian matrix: the nonzeros for column *i* (with *i* = 1 for the first column) are in J[j] for colstarts[*i*-1] - 1 $\le j \le$ colstarts[*i*] - 2, which looks more natural in Fortran notation: the calling sequences are compatible with the *f*2*c* calling conventions for Fortran.

Bounds are conveyed in boundc_ as follows:

boundc_[0] is the value passed for ∞ ;

boundc_ + 1 is an array of lower and upper bounds on the variables, and

boundc_ + $2*n_var$ + 1 is an array of lower and upper bounds on the constraint bodies. The initial guess appears in x0comn_. Bounds of $\pm \infty$ are rendered as 1.7e308 and -1.7e308.

The -f command-line option causes nlc to emit Fortran 77 equivalents of feval_ and ceval_; they correspond to the Fortran signatures

```
double precision function feval(nobj, needfg, x, g)
integer nobj,needfg
double precision x(*), g(*)
```

and

```
subroutine ceval(needfg, x, c, J)
integer needfg
double precision x(*), c(*), J(*)
```

and the auxiliary arrays are rendered as the COMMON blocks

```
common /funcom/ nvar, nobj, ncon, nzc, densej, colrow
integer nvar, nobj, ncon, nzc, densej, colrow(*)
common /boundc/ bounds
double precision bounds(*)
common /x0comn/ x0
double precision x0(*)
common /auxcom/ nlc
integer nlc ! number of nonlinear constraints
```

where the *'s have the values described above. (Strictly speaking, it would be necessary to make problemspecific adjustments to the dimensions in other Fortran source that referenced these common blocks, but most systems follow the rule that the array size seen first wins, in which case it suffices to load the object for feval and ceval first.) The first nobj values of the colrow array have value 0 or 1 to indicate whether the corresponding objective is to be minimized (0) or maximized (1).

Command-line option -1 causes nlc to emit variants feval0_ and ceval0_ of feval_ and

ceval_ that omit gradient computations. They have signatures

real feval0_(fint *nobj, real *x); void ceval0 (real *x, real *c);

With command-line option -3, nlc produces all four routines (or, if -f is also present, equivalent Fortran).

Writing *stub*.nl files for debugging

You can use AMPL's write command or its -o command-line flag to get a *stub*.nl (and any other needed auxiliary files) for use in debugging. Normally AMPL writes a binary-format *stub*.nl, which corresponds to a command-line -ob*stub* argument. Such files are faster to read and write, but slightly less convenient for debugging, in that write_sol notes the format of *stub*.nl (binary or ASCII — by looking at binary_nl) and writes *stub*.sol in the same format. To get ASCII format files, either issue an AMPL write command of the form

write gstub;

or use the *-ogstub* command-line option. Your solver should see exactly the same problem, and AMPL should get back exactly the same solution, whether you use binary or ASCII format *stub*.nl and *stub*.sol files (if your computer has reasonable floating-point arithmetic).

With AMPL versions \geq 19970214, binary *stub*.nl files written on one machine with binary IEEE-arithmetic can be read on any other.

Use with MATLAB[®] or Octave

It is easy to use AMPL with MATLAB or Octave. This requires the help of a *mex* file that reads *stub*.nl files, writes *stub*.sol files, and provides function, gradient, and Hessian values. Example file amplfunc.c is source for an amplfunc.mex that looks at its left- and right-hand sides to determine what it should do and works as follows:

[x,bl,bu,v,cl,cu] = amplfunc('stub')

or

```
[x,bl,bu,v,cl,cu,cv] = amplfunc('stub')
```

reads stub.nl and sets

```
x = primal initial guess,
```

- bl = lower bounds on the primal variables,
- bu = upper bounds on the primal variables,
- v = dual initial guess (often a vector of zeros),
- cl = lower bounds on constraint bodies,
- cu = upper bounds on constraint bodies, and (when present)
- cv = variables complementing constraints:

cv[i] > 0 means constraint *i* complements variable cv[i] - 1.

[f,c] = amplfunc(x,0)

sets

f = value of first objective at *x* and

c = values of constraint bodies at x.

```
[g,Jac] = amplfunc(x,1)
```

sets

g = gradient of first objective at x and Jac = Jacobian matrix of constraints at x.

W = amplfunc(Y)

sets W to the Hessian of the Lagrangian (equation (*) in the section "Evaluating Nonlinear Functions" above) for the first objective at the point x at which the objective and constraint bodies were most recently evaluated. Finally,

$$[] = amplfunc(msg, x, v)$$

calls write_sol(msg, x, v, 0) to write the stub.sol file, with

- msg = termination message (a string),
- \mathbf{x} = optimal primal variables, and
- v = optimal dual variables.

It is often convenient to use .m files to massage problems to a desired form. To illustrate this, the examples directory offers the following files (which are simplified forms of files used in joint work with Michael Overton and Margaret Wright):

• init.m, which expects variable pname to have been assigned a *stub* (a string value), reads *stub*.nl, and puts the problem into the form

minimize f(x)

s.t.
$$c(x) = 0$$

and $d(x) \ge 0$.

For simplicity, the example init.m assumes that the initial x yields d(x) > 0. A more elaborate version of init.m is required in general.

• evalf.m, which provides [f,c,d] = evalf(x).

• evalg.m, which provides [g, A, B] = evalg(x), where A = c'(x) and B = d'(x) are the Jacobian matrices of c and d.

• evalw.m, which computes the Lagrangian Hessian, W = evalw(y, z), in which y and z are vectors of Lagrange multipliers for the constraints

c(x) = 0

and

 $d(x) \geq 0$,

respectively.

• enewt.m, which uses evalf.m, evalg.m and evalw.m in a simple, non-robust nonlinear interior-point iteration that is meant mainly to illustrate setting up and solving an extended system involving the constraint Jacobian and Lagrangian Hessian matrices.

• savesol.m, which writes file *stub*.sol to permit reading a computed solution into an AMPL session.

• hs100.amp, an AMPL model for test problem 100 of Hock and Schittkowski [15].

• hs100.nl, derived from hs100.amp. To solve this problem, start MATLAB and type

```
pname = 'hs100';
init
enewt
savesol
```

Amplfunc.c provides dense Jacobian matrices and Lagrangian Hessians; spamfunc.c is a variant that provides sparse Jacobian matrices and Lagrangian Hessians. To see an example of using spamfunc, change all occurrences of "amplfunc" to "spamfunc" in the .m files.

5. Utility Routines and Interface Conventions

-AMPL Flag

Sometimes it is convenient for a solver to behave differently when invoked by AMPL than when invoked "stand-alone". This is why AMPL passes a string that starts with -AMPL as the second command-line argument when it invokes a solver. As a simple example, nl2l.c turns dn2gb's default printing off when it sees -AMPL, and it only invokes write_sol when this flag is present.

Conveying solver options

Most solvers have knobs (tolerances, switches, algorithmic options, etc.) that one might want to turn. An AMPL convention is that appending _options to the name of a solver gives the name of an environment variable (AMPL option) in which the solver looks for knob settings. Thus a solver named wondersol would take knob settings from \$wondersol_options (the value of environment variable wondersol_options). For interactive use, it's usually a good idea for a solver to print its name and perhaps version number when it starts, and to echo nondefault knob settings to confirm that they've been seen and accepted. It's also conventional for the msg argument to write_sol to start with the solver's name and perhaps version number. Since AMPL echoes the write_sol's msg argument when it reads the solution, a minor problem arises: if there are no nondefault knob settings, an interactive user would see the solver's name printed twice in a row. To keep this from happening, you can set need_nl (i.e., asl->i.need_nl_) to a positive value; this causes write_sol to insert that many backspace characters at the beginning of *stub*.sol. Usually this is done as follows: initially you execute, e.g.,

need_nl = printf("wondersol 3.2: ");

(Note that printf returns the number of characters it transmits — exactly what we need.) Subsequently, if you echo any options or otherwise print anything, also set need_nl to 0.

Conventionally, $solver_options$ may contain keywords and name-value pairs, separated by white space (spaces, tabs, newlines), with case ignored in names and keywords. For name-value pairs, the usual practice is to allow white space or an = (equality) sign, optionally surrounded by white space, between the name and the value. For debugging, it is sometimes convenient to pass keywords and name-value pairs on the solver's command line, rather than setting $solver_options$ appropriately. The usual practice is to look first in $solver_options$, then at the command-line arguments, so the latter take precedence.

Interface routines getstub, getopts, and getstops facilitate the above conventions. They have apparent prototypes

```
char *getstub (char ***pargv, Option_Info *oi);
int getopts (char **argv, Option_Info *oi);
char *getstops(char ***pargv, Option_Info *oi);
```

which you can import by saying

```
include "getstub.h"
```

rather than (or in addition to)

include "asl.h"

Type Option_Info is also declared in getstub.h; it is a structure whose initial components are

```
char *sname;
                     /* invocation name of solver */
                    /* solver name in startup "banner" */
char *bsname;
char *opname;
                    /* name of solver_options environment var */
keyword *keywds;
                    /* key words */
int n_keywds;
                    /* number of key words */
int want_funcadd;
                   /* whether funcadd will be called */
char **usage;
char *version;
                    /* for -v and Ver key ASL() */
                    /* solver-specific usage message */
Solver_KW_func *kwf; /* solver-specific keyword function */
```

Fileeq_func *feq;	/*	for n=filename */					
keyword *options;	/*	command-line options	(with	-)	before	stub	*/
int n_options;	/*	number of options */					

Ordinarily a solver declares

static Option_Info Oinfo = { ... };

and supplies only the first few fields (in place of "..."), relying on the convenience of static initialization setting the remaining fields to zero.

- 30 -

Function getstub looks in *pargv for the *stub*, possibly preceded by command-line options that start with "-"; getstub provides a small default set of command-line options, which may be augmented or overridden by names in oi->options. Among the default command-line options are '-?', which requests a usage summary that reports oi->sname as the invocation name of the solver; '-=', which summarizes possible keyword values; -v, which reports the versions of the solver (supplied by oi->version) and of amplsolver.a (which is available in cell ASLdate_ASL, declared in asl.h); and, if oi->want_funcadd is nonzero, -u, which lists the available imported functions; imported functions are discussed in their own section above. If it finds a *stub*, getstub checks whether the next argument begins with -AMPL and sets amplflag accordingly; if so, it executes

if (oi->bsname)
 need_nl = printf("%s: ", oi->bsname);

At any rate, it sets *pargv to the command-line argument following the *stub* and optional -AMPL and returns the *stub*. It returns 0 (null) if it does not find a *stub*.

Function getopts looks first in \$*solver_options*, then at the command line for keywords and optional values; oi->opname provides the name of the *solver_options* environment variable. Getopts is separate from getstub because sometimes it is convenient to call jacOdim, do some storage allocation, or make other arrangements before processing the keywords. For cases where no such separation is useful, function getstops calls getstub and getopts and returns the *stub*, complaining and exiting if none is found.

Keywords are conveyed in keyword structures declared in getstub.h:

```
typedef struct keyword keyword;
typedef char *Kwfunc(Option_Info *oi, keyword *kw, char *value);
struct keyword {
    char *name;
    Kwfunc *kf;
    void *info;
    char *desc;
    };
```

Array oi->keywds describes oi->n_keywds keywords that may appear in \$*solver_options*; these keyword structures must be sorted (with comparisons as though by strcmp) on their name fields, which must be in lower case. Similarly, oi->options is an array of oi->n_options keywords for initial command-line options, which must also be sorted; often oi->n_options = 0. The desc field of a keyword may be null; it provides a short description of the keyword for use with the -= command-line option. If desc starts with an = sign, the text in desc up to the first space is appended to the keyword in the output of the -= command-line option. The kf field provides a function that processes the value (if any) of the keyword. Its arguments are oi (the Option_Info pointer passed to getstub), a pointer kw to the keyword structure itself, and a pointer value to the possible value for the keyword (stripped of preceding white space). The kf function may use kw->info as it sees fit and should return a pointer to the first character in value that it has not consumed. Ordinarily getopts echoes any keyword assignments it processes (and sets need_nl = 0), but the kf function can suppress this echoing for a particular assignment by executing

DRAFT FOR COMMENT

oi->option_echo &= ~ASL_OI_echothis;

or for all subsequent assignments by executing

oi->option_echo &= ~ASL_OI_echo;

name	description of value		
CK_val	known character value in known place		
C_val	character value in known place		
DA_val	real (double) value in asl		
DK_val	known real (double) value in known place		
DU_val	real (double) value: offset from uinfo		
D_val	real (double) value in known place		
IA_val	int value in asl		
IKO_val	int value 0 in known place		
IK1_val	int value 1 in known place		
IK_val	known int value in known place		
IU_val	int value: offset from uinfo		
I_val	int value in known place		
LK_val	known Long value in known place		
LU_val	Long value: offset from uinfo		
L_val	Long value in known place		
SU_val	short value: offset from uinfo		
Ver_val	report version		
WS_val	set wantsol in Option_Info		
Table 9. know and functions in get stub b			

- 31 -

For convenience, amplsolver.a provides a variety of keyword-processing functions. Table 9 summarizes these functions; their prototypes appear in getstub.h, which also provides a macro, nkeywds, for computing the n_keywds field of an Option_Info structure from a keyword declaration of the form

```
static keyword keywds[] = { ... };
```

To allow compilation by a K&R C compiler, it is best to cast the info fields to (Char*) (which is (char*) with K&R C and (void*) with ANSI/ISO C and C++). Often it is convenient to use macro KW, defined in getstub.h, for this. An example appears in file tnmain.c, in which the keywds declaration is followed by

```
static Option_Info Oinfo =
    { "tn", "TN", "tn_options", keywds, nkeywds, 1 };
```

Many other examples appear in various subdirectories of *netlib*'s ampl/solvers directory. Occasionally it is necessary to make custom keyword-processing functions, as in the example files keywds.c, rvmsg.c and rvmsg.h, which are discussed further below.

Some solvers, such as minos and npsol, have their own routines for parsing keyword phrases. For such a solver you can initialize oi->kwf with a pointer to a function that invokes it; if getopts sees a keyword that does not appear in oi->keywds, it changes any underscore characters to blanks and passes the resulting phrase to oi->kwf. Some solvers, such as minos, also need a way to associate Fortran unit numbers with file names; oi->feq (if not null) points to a function for doing this. See ampl/solvers/minos/m55.c for an example that uses all 12 of the Option_Info fields shown above, including oi->kwf and oi->feq.

Many solvers allow outlev to appear in \$*solver_options*. Generally, outlev = 0 means "no printed output", and larger integers cause the solver to print more information while they work. Another common keyword is maxit, whose value bounds the number of iterations allowed. For stand-alone

invocations (those without -AMPL), solvers commonly recognize wantsol=n, where n is the sum of

- 1 to write a . sol file,
- 2 to print the primal variable values,
- 4 to print the dual variable values, and
- 8 to suppress printing the solution message.

A special keyword function, WS_val, processes wantsol assignments, which are interpreted by write_sol. Strings WS_desc_ASL and WSu_desc_ASL provide descriptions of wantsol for constrained and unconstrained solvers, respectively, and appear in many of the sample drivers available from *netlib*.

Printing and Stderr

To facilitate using AMPL and solvers in some contexts, such as some versions of Microsoft Windows, it is best to route all printing through printf and fprintf. Because of this, and because some systems furnish a sprintf that does not give the return value specified by ANSI/ISO C, amplsolver.a provides suitable versions of printf, fprintf, snprintf, sprintf, vfprintf, vsnprintf, and vsprintf that function as specified by ANSI/ISO C, except that they do not recognize the F, L, j, ll, t, or z qualifiers or the %n format item; as in AMPL, they provide some extensions: they turn %.0g and %.0G into the shortest decimal string that rounds to the number being converted, and they allow negative precisions for %f. These provisions apply to systems with IEEE, VAX, or IBM mainframe arithmetic, and comments in solvers/makefile explain how to use the system's printf routines on other systems.

On systems where it is convenient to redirect stderr, it is best to write error messages to stderr. Unfortunately, redirecting stderr is inconvenient on some systems (e.g., Microsoft systems with the usual Microsoft shells). To promote portability among systems, amplsolver.a provides access to

```
extern FILE *Stderr,
```

which can be set, as appropriate, to stderr or stdout. Thus we recommend writing error messages to Stderr rather than stderr, as is illustrated in various examples discussed above.

Formatting the optimal value and other numbers

An AMPL convention is that solvers should report (in the msg argument to write_sol) the final objective value to \$objective_precision significant figures. Interface routines g_fmtop and obj_prec facilitate this. They have apparent prototypes

int g_fmtop(char *buf, double v); int obj_prec(void);

For use as the "*" argument in the format %.*g, obj_prec returns <code>\$objective_precision</code>. Occasionally it may be convenient to use <code>g_fmtop</code> instead. It stores the appropriate decimal approximation in buf (using the same conversion routine as AMPL's printing commands), and returns the number of characters (excluding the terminating null) it has stored in buf. The end of nl2l.c illustrates both the use of <code>g_fmtop</code> and of the Sprintf in amplsolver.a. The latter is there because, contrary to standard (ANSI/ISO) C, the sprintf on some systems does not return the count of characters written to its first argument. Ordinarily, Sprintf is the sprintf described above in the section "Printing and stderr", but if you are using the system's sprintf, then Sprintf is similar to sprintf, but only understands <code>%c</code>, <code>%d</code>, <code>%ld</code>, and <code>%s</code> (and complains if it sees something else).

Two relatives of g_fmtop that are also in amplsolver.a are

int g_fmt(char *buf, double v); int g_fmtp(char *buf, double v, int prec);

g_fmtp rounds its argument to prec significant figures unless prec is 0, in which case it stores in buf the shortest decimal string that rounds to v (provided the machine uses IEEE, VAX, or IBM mainframe arithmetic: see [10]); g_fmt(buf,v) = g_fmtp(buf,v,0).

If they find an exponent field necessary, both g_fmtop and its relatives delimit it with the current value of

extern char g_fmt_E;

(whose declaration appears in asl.h). The default value of g_fmt_E is 'e'.

By default, g_fmtop and its relatives only supply a decimal point if it is followed by a digit, but if you set

extern int g_fmt_decpt;

(declared in asl.h) to a nonzero value, they always supply a decimal point when v is finite. If you set g_fmt_decpt to 2, these routines supply an exponent field for finite v. The nlc program discussed above uses these features when it writes Fortran.

A "Solver" for Gradients and Hessians: gjh

File examples/gjh.c is source for a "solver" that computes objective and constraint gradients and the Lagrangian Hessian at the current (primal and dual) point and writes them to a file that can be read in an AMPL session (via "include filename" or "model filename;") to make these first and second derivative values available as AMPL params. The solve_message gives the filename as well as a command for removing the file after reading it.

More examples

Some examples illustrating the above points appear in the solvers/examples directory. One such example is tnmain.c, a wrapper for Stephen Nash's LMQN and LMQNBC [18,17], which solve unconstrained and simply bounded minimization problems by a truncated Newton algorithm. Since tnmain.c calls getstub, the resulting solver, tn, explains its usage when invoked

tn '-?'

and summarizes the keywords it recognizes when invoked

tn '-='

For another example, files mng.c and nl2.c are for solvers called mng and nl2, which are more elaborate variants of the mngl and nl21 considered above (source files mngl.c and nl21.c). Both use auxiliary files keywds.c, rvmsg.c and rvmsg.h to turn the knobs summarized in [11] and pass a more elaborate msg to write_sol. Their linkage, in examples/makefile, also illustrates adding imported functions, which we will discuss shortly. Unlike mngl, mng checks to see if the objective is to be maximized and internally negates it if so.

File mnh.c is a variant of mng.c that supplies the analytic Hessian matrix computed by duthes to solver mnh, based on PORT routine dmnhb. For maximum likelihood problems, it is sometimes appropriate to use the Hessian at the solution as an estimate of the variance-covariance matrix; mnh offers the option of computing standard-deviation estimates for the optimal solution from this variance-covariance matrix estimate. Specify stddev=1 in \$mnh_options or on the command line to exercise this option, or specify stddev_file=*filename* to have this information written to a file.

Various subdirectories of

http://ampl.com/netlib/ampl/solvers/

provide other examples of drivers for linear and nonlinear solvers. See

http://ampl.com/netlib/ampl/solvers/README

for more details.

Evaluation Test Program

File et.c is source for program *et* (*evaluation tester*) for testing various kinds of ASL evaluations. It can use the various readers to read specified *stub*.nl files, print and change the current primal and dual variable values, compute objective function and constraint bodies, their derivatives, Lagrangian Hessians and Hessian-vector products, and use finite differences to check compute derivatives. The *et* program reads commands from the standard input or a file or files given on the command line and produces output in response to them. After invoking et, type a question mark and carriage return to see a detailed usage summary, or invoke

et -?

or

et --help

for a brief usage summary.

Multiple problems and multiple threads

It is possible to have several problems in memory at once, each with its own ASL pointer. To free the memory associated with a particular ASL pointer asl, execute

ASL_free(&asl);

this call sets asl = 0. To allocate problem-specific memory that will be freed by ASL_free, call Mlalloc rather than Malloc. Do not pass such memory to realloc or free.

Variant solvers2 of the solvers directory, with source

http://ampl.com/netlib/ampl/solvers2.tgz

is designed for use with multiple threads — and for large nonlinear problems is often more efficient than the facilities in the solvers directory. For using solvers or solvers2 with multiple threads, amplsolver.a should be compiled with ALLOW_OPENMP #defined if *OPENMP* is available, or with MULTIPLE_THREADS #defined along with suitable #define ACQUIRE_DTOA_LOCK(*n*) and FREE_DTOA_LOCK(*n*) directives to provide exclusive access to a few short critical regions (with distinct values of *n*). A possible approach is first to create arith.h by saying "make arith.h", then to add

#define ALLOW OPENMP

or else

#define MULTIPLE_THREADS

and suitable definitions of ACQUIRE_DTOA_LOCK(*n*) and FREE_DTOA_LOCK(*n*) to the end of arith.h, and finally to create amplsolver.a by saying "make".

With solvers2, each thread can use its own *EvalWorkspace* pointer ew, acquired by invoking apparent function

EvalWorkspace *ew = ewalloc();

The problem-specific functions, such as objval() and objgrd() discussed above have equivalent thread-specific forms with _ew appended to the function name and ew as the first argument, e.g.,

```
real objval_ew(EvalWorkspace *ew, real *x);
real objvale_ew(EvalWorkspace *ew, real *x, fint *nerror);
int xknown_ew(EvalWorkspace *ew, real *X)
int xknowne_ew(EvalWorkspace *ew, real *X, fint *nerror)
```

see solvers2/asl.h for more details.

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