



Purpose:

Minimization of optics of existed separators First step: quad fields v.9.10.100 from 05/22/15

1. Introduction

2. New Block "Fitting constraints"

3. Selecting a block to minimize

4. Run minimization

5. Examples

6. levmar example

Recently the first stage of optics minimization procedure was introduced, based on the "levmar" package by M.I.A. Lourakis using the Levenberg-Marquardt nonlinear least square algorithm. At this stage only the quadrupole fields can be varied to minimize user constraints for matrix and beam ellipse elements. In the future this minimization procedure will be used to define curved profile shape, fragment spatial distributions in Monte Carlo mode, and optimize intensity/purity combination.

Based on

levmar: Levenberg-Marquardt nonlinear least squares algorithms in C/C++. M.I.A. Lourakis July 2004. http://users.ics.forth.gr/~lourakis/levmar

Minimization for

- E-blocks (extended configurations)
- with non-linked matrices
- set the option "Allow remote matrices recalculation"



users.ics.forth.gr/~lourakis/levmar/

levmar : Levenberg-Marquardt nonlinear least squares algorithms in C/C++

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If you are looking for a general-purpose <u>sparse</u> Levenberg-Marquardt C/C++ implementation, please have a look at <u>sparseLM</u>.

Introduction

This site provides <u>GPL</u> native ANSI C implementations of the <u>Levenberg-Marguardt optimization algorithm</u>, usable also from C++, <u>Matlab</u>, <u>Perl</u>, <u>Python</u>, <u>Haskell</u> and <u>Tcl</u> and explains their use. Both <u>unconstrained</u> and <u>constrained</u> (under linear equations, inequality and box constraints) Levenberg-Marguardt variants are included. The <u>Levenberg-Marguardt</u> (LM) algorithm is an iterative technique that finds a local minimum of a function that is expressed as the sum of squares of nonlinear functions. It has become a standard technique for nonlinear least-squares problems and can be thought of as a combination of <u>steepest descent</u> and the <u>Gauss-Newton</u> method. When the current solution is far from the correct one, the algorithm behaves like a steepest descent method: slow, but guaranteed to converge. When the current solution is close to the correct solution, it becomes a Gauss-Newton method.

Technical Overview

Levmar includes double and single precision LM C/C++ implementations, both with analytic and finite difference approximated Jacobians. It is provided free of charge, under the terms of the <u>GNU General</u> <u>Public License</u>. The mathematical theory behind unconstrained Levmar is described in detail in the lecture notes entitled <u>Methods for Non-Linear Least Squares Problems</u>, by K. Madsen, H.B. Nielsen and O. Tingleff, Technical University of Denmark; <u>Matlab implementations</u> of the algorithms presented in the lecture notes are also available. Note however that the formulation of the minimization problem adopted here is slightly different from that described in the <u>lecture notes</u>. There is also a <u>short note</u>, providing a quick overview of the material in the lecture notes.

To deal with linear equation constraints, levmar employs variable elimination based on QR factorization, as described in ch. 15 of the book <u>Numerical Optimization</u> by Nocedal and Wright. For the box-constrained case, levmar implements the algorithm proposed by C. Kanzow, N. Yamashita and M. Fukushima, <u>Levenberg-Marguardt methods for constrained nonlinear equations with strong local convergence properties</u>, Journal of Computational and Applied Mathematics 172, 2004, pp. 375-397.

levmar provides the following two options regarding the solution of the linear systems formed by the augmented normal equations:

1. If you have LAPACK (or an equivalent vendor library such as Intel's MKL, AMD's AMCL, Sun's performance library, IBM's ESSL, SGI's SCSL, NAG, ...), the included LAPACK-based solvers can be used. This is the default option. The employed solver is based on the LU decomposition. Additionally, for experimenting with other approaches, linear solvers based on the Cholesky and QR decompositions have been supplied.

2. If LAPACK is unavailable, a LAPACK-free, LU-based linear systems solver can be used by undefining HAVE LAPACK in levmar.h.

- Unconstrained optimization
 - o dlevmar_der(): double precision, analytic Jacobian
 - o dlevmar_dif(): double precision, finite difference approximated Jacobian
 - o slevmar_der(): single precision, analytic Jacobian
 - o slevmar_dif(): single precision, finite difference approximated Jacobian

Constrained optimization

- o dlevmar_lec_der(): double precision, linear equation constraints, analytic Jacobian
- o dlevmar_lec_dif(): double precision, linear equation constraints, finite difference approximated Jacobian
- o slevmar_lec_der(): single precision, linear equation constraints, analytic Jacobian
- slevmar_lec_dif(): single precision, linear equation constraints, finite difference approximated Jacobian

o dlevmar bc der(); double precision, box constraints, analytic Jacobian

- odlevmar_bc_dif(): double precision, box constraints, finite difference approximated Jacobian
- o slevmar_bc_der(): single precision, box constraints, analytic Jacobian
- o slevmar_bc_dif(): single precision, box constraints, finite difference approximated Jacobian
- dlevmar_blec_der(): double precision, box & linear equation constraints, analytic Jacobian
- dlevmar_blec_dif(): double precision, box & linear equation constraints, finite difference approximated Jacobian
- o slevmar_blec_der(): single precision, box & linear equation constraints, analytic Jacobian
- slevmar_blec_dif(): single precision, box & linear equation constraints, finite difference approximated Jacobian
 - o dlevmar_bleic_der(): double precision, box, linear equation & inequality constraints, analytic Jacobian
 - o dlevmar_bleic_dif(): double precision, box, linear equation & inequality constraints, finite difference approximated Jacobian
 - o slevmar_bleic_der(): single precision, box, linear equation & inequality constraints, analytic Jacobian
 - slevmar_bleic_dif(): single precision, box, linear equation & inequality constraints, finite difference approximated Jacobian





OT, 26-May-2015, East Lansing





LISE++

- 1. Select a optical block to minimize, Check in a parameter to minimize, Set bounds constraint
- 2. Create a block "Fitting constraints" Set constraints

3. Run minimization



Comn	nand			
5. <u>01</u>	"q1B "	0.7	<u>-1.86164</u>	9.75;

Command 10.0 "fit1" -2. 6. 0.0 .001 ;

3. Run minimization



files\examples\NSCL\ A1900_extended_LISE_FIT.lpp

The next file is to append standard constraint blocks files\examples\ **FITconstraints.lpp**



Introduction: information about blocks used for minimization



First order matrix elements : View & Print

Optics settings : FAST EDITING Optics settings : View & Print or



-	Optio	cs setting	gs (fast editing)												
BI	ock		Given Name	Start(m)	Length(m)	B0(kG)	Br(Tm)cor/*real	DriftM/*Angle	Rapp(cm)/*R(. Leff(m)/*Ldip(m)	2 nd order	CalcMatr/*Z-Q	AngAcc,Apps,Sli	B COSY Fit	BE [•
d		drift	z089	28.783	0.5640			standard					- HV	•	е	
D	-	= Dipole	D4	29.347	2.4300	+9.6965	* 3.0000	* +45.0	* 3.0939	* 2.4299	yes	* O	- HV		S	
d		drift	z097	31.777	0.5260			standard					- HV		е	
F	* F	Fit	sigY	32,303	0.0000									s3 < 50	е	
Q	◇ <	(Quad>	Q098-8TA	32,303	0.4300	+7.0851	3.0000	QUAD	15.0000	0.4300	yes	1 R	- HV	FIT	е	
F	* F	Fit	sigY	32,733	0.0000									s3 < 50	е	
d		drift	z099	32.733	0.1720			standard					- HV		е	
Q	◇ <	(Quad>	Q100-8TB	32,905	0.7480	-8.1167	3.0000	QUAD	13.3000	0.7480	yes	1 R	- HV	FIT	е	
F	* F	Fit	sigY	33.653	0.0000									s3 < 50	е	
d		drift	z101	33.653	0.1756			standard					- HV		е	
Q	♦	(Quad>	Q102-8TC	33.828	0.7480	+4.2117	3.0000	QUAD	13.3000	0.7480	yes	1 R	- HV	FIT	е	
F	* F	Fit	sigY	34.576	0.0000									s3 < 50	е	
d		drift	z103	34.576	0.3750			standard					- HV		е	
d		drift	z104	34.951	0.4320			standard					- HV		е	
F	* F	Fit	focusX	35.383	0.0000									R12 = 0	е	
F	* F	Fit	focusY	35.383	0.0000									R34 = 0	е	
F	* F	Fit	X-dispers	35.383	0.0000									R16 = 0	е	
F	* F	Fit	T-dispers	35.383	0.0000									R26 = 0	е	
F	* F	Fit	sigmaX	35.383	0.0000									s1 < 2	е	_
F	* F	Fit	sigmaY	35.383	0.0000									s3 < 1	е	
S	I	_slits_	Image4(105)	35.383	0.0000			SLITS					HV		е	
d		drift	z105	35.383	0.3490			standard							е	
d		drift	z106	35.732	0.0890			standard						100 A.	е	-
-9	Selec	ted block:					[- Angular accepta	ance (mrad) —	- Inside Aperture (mm)		-Slits (mm) after this		1-st order Matrix E	lement:	s –
		Dispers	ive (M-dinole)	_	Block	Selecte	d Block Edit		Use	min m	nax Use	min	max Use	A Matrix P	lot	
11		Dispore	ine (in dipole)	Le	ngth [m]	NHV		Horizontal ±		X = -50 5	0	X =		1 Manx I	01	-
	Letic	all automa	atically 🔲	1 0	.0001	Mutli	pole Edit	Vertical ±		Y= -50 5		Y =	── ┌ .	Beam-Sigma	a Plot	
	Block	k name =	tuning	Len this l	gth after block [m]	🜒 🚺 Cuts (Ac	cceptances)	_ Shape		_ Shape		Shape		6'o' View		
(Charg	ge State (2	Z-Q) = 0	0	.0001	රං Optic	al Matrix	Rectangle C	Ellipse	Rectangle C 📀	Ellipse	Rectangle 🔎	C Ellipse	🗸 Quit 💡	Help	



New Optic Block "Fitting Constraints"



- spectrometer d	esign				
Block	Given Name	Z-Q Length,m	Enable	- Insert Mode	Insert block
🍳 🔷 <quad></quad>	Q041-3TB	0.812	+	G hafan	Materiale
d 🔲 drift	z042	0.136	+	ve berore	Materiais
🍳 🔷 <quad></quad>	Q043-3TC	0.43	+	C after	W Vedge Target
d 🔲 drift	z044	0.563	+		
🚬 = Dipole	D2	0 2.43	+	Move element	Matenal(Detector)
d 🔲 drift	z052	0.552	+		A Faraday cup
🍳 🔷 <quad></quad>	Q053-4TA	0.43	+		
d 🔲 drift	z054	0.17	+	🕂 Down	
🍳 🔷 <quad></quad>	Q055-4TB	0.732	+		- Optical
d 🔲 drift	z056	0.176	+		
🍳 🔷 <quad></quad>	Q057-4TC	0.526	+	👯 Edit	dispersive non-dispersive
d 🔲 drift	z058	0.658	+	Y Delete	
S 👖 _slits_	Image2(059)	0	+	► Delete	Dispersive (M-dipole)
🛛 🔻 Wedge	Wedge		+		Wien velocity filter R Beam Rotation
d 🔲 drift	z060	0.658	+	🖌 ок	
🝳 🔷 <quad></quad>	Q062-5TA	0.526	+	•	Eectrostatic dipole
d 🔲 drift	z063	0.176	+	7 Help	G 🔢 Gas-filled separator
Q 🔷 <quad></quad>	Q064-5TB	0.732	+		
d 🔲 dift	2065	0.17	+		Compensating Dipole
- Selected block				- Total	special
Enable 🔽	1	Dispersive (M-dipole)		Blocks	dispersive RF-based (no beam dinamics changes)
Let call automatic	ally 🗆	Block Length [m]	0.0001	82	K + REconcrator Z Delay (officience) blood
Block name = tur	ning	Length after this block [m]	0	Length [m]	
Charge State 17-0	n = 0	Sequence number	3	35.821	B ■ RF buncher F * Fitting constraints
5.13.95 51010 (E G	0				

sigY		— ×
Desired parameters of element to fit	Select Element to Fit	
Constraint : Upper limit is	- Global Block matrix	Beam (sigmas)
50	1. X C 29295 C -0.5429 C O C O C O C O	C 4.3808 [mm]
Desired Value = 30	2. T C 1.5168 C 0.0604 C 0 C 0 C 0 C 0	C 1.5595 [mrad]
Desired Accuracy =	3, Y C 0 C 0 C 27.8909 C 3.0216 C 0 C 0	(* 36.9083 [mm]
Constraint name = sigY	4. F C 0 C 0 C 25.4445 C 2.7207 C 0 C 0	C 33.4838 [mrad]
	5. L C -0.0014 C 0.0006 C 0 C 0 C 1 C -10.8848	C 0.7619 [mm]
TRANSPORT notification		C 0.07 [%]
10.2 3.3.50 1 "sigY"	/[mm] /[mrad] /[mm] /[mrad] /[mm] /[%]	Dimension
	Det = 1.00074	Dimension
🖌 OK 🗙 Cancel 🤶 Help	Typical TRANSPORT constraints	mm (+ t cm





6

42* possible selection for global matrix elements and beam sigma vector

The "Fit constraint" dialog. For a constraint the user selects an element from an optical matrix or beam sigma vector, and set its desired value and precision (weight).

(some matrix elements can be disabled if non rotation or solenoid blocks)

Desired parameters of element to fit Constraint : Upper limit is Desired Value = 50 Desired Accuracy = 1	Select Element to Fit Global Block matrix 1. × C 2.9295 C -0.5423 2. T C 1.5168 C 0.0604 3. × C 0 C 0		Beam (sigmas) C 4.3808 [mm] C 1.5595 [mrad] C 36.9083 [mm]		
Constraint name = sigY TRANSPORT notification 10.2 3. 3. 50 1 "sigY" OK Cancel 7 Help	4. F C 0 C 0 5. L C -0.0014 C 0.0006 6. D C 0 C 0 /[mm] /[mrad Det = 1.00074	3. Y 0 0 0 -27.8909 -3.0216 0 0 0 4. F 0 0 0 25.4445 2.7207 0 0 0 5. L 0 0 0 0 0 0 1 0.088 6. D 0 0 0 0 0 0 1 10.88 bet = 1.00074 /(mm) /(mm) /(mm) /(mm) /(mm) /(% Typical TRANSPORT constraints			
		Typical TRANSPORT constraints Zoom In Zoom Out			
to limit is Inverse wei limit is	ght	Desired optical condition Point to point imaging:	Typical fitting constraint		
\downarrow		Horizontal plane $R(12) = 0$ Vertical plane $R(34) = 0$	101. 2. 00001 'F1'; 103. 4. 00001 'F2';		
ANSPORT notification of selected	constraint. levelopment	Parallel to point focus: Horizontal plane $R(11) = 0$ Vertical plane $R(33) = 0$	101. 1. 00001 'F3';		
		Vertical plane R(55) = 0	105. 5. 00001 14,		



Special LISE⁺⁺ **functions fore limit constraints**





Levmar functions for "equal_to" constraints are used. Important to have limit constraints in LISE⁺⁺ for apertures New Functions should continuous!





In current version only M-Quad B-fields and E-Quad voltages

Set in it!



No matrix link to external file!



Optimization dialog

Μ	IC	CΗ	110	37	١N	S	T	AT	Ē
U	Ν	T	۷	Ε	R	s	I	Т	γ
I	6	I		5	I	£,			Þ

Experiment Settings Physics Models	Calculations	Utilities	1D-Plot	2D-Plot	Databases	Help
Projectile						
Target						
Stripper after Target						
Spectrometer Design	_					
Optics		Tune	spectromet	er for settin	g fragment o	n beam axis
Gamma registration		Tune	spectromet	er for settin	g fragment a	t middle of slit
Setting Fragment		OPTI	MIZATION	(optical eler	nent parame	ters fitting)
Tune spectrometer for the primary	beam	Manu	ial recalcula	tion of e-bl	ocks matrices	(only for Experts!)
		Updat	te matrices	linked with	COSY files	
		Envel	ope plot			

First order matrix elements : Plot First order matrix elements : View & Print Optics settings : FAST EDITING Optics settings : View & Print Brho(Erho) Analyzer The First- and Second-Order Matrix Elements for an Ideal Magnet

The "Optics Fit" dialog. The left panel shows optical blocks with varying parameters, whereas blocks with fitting constraints.

Optics fit	
Blocks with parameters to vary	Constraint blocks
#01 Position@055: Q084-7TA #02 Position@057: Q086-7TB #03 Position@059: Q088-7TC #04 Position@064: Q098-8TA #05 Position@067: Q100-8TB #06 Position@070: Q102-8TC	#01 Position@063: \$3 < 50
N iter = 500	
Fit Previuos values	Fit Settings Matrix Plot
	Browse output file 🛛 📐 Beam-Sigma Plot
? Help	t4.11t

evmar minimization settings							
Options				- LevMar package samples			
Maximum number of iterations = 500 Use Lower & Upper bounds ✓ (0-15) (% Run minimization							
- Stopping threst	nolds			- Louikier peokeen info			
Options	Value	Stopping threshold	Default value	LEVMAR :			
tau	1.00e-03	mu/max[J^T J]_ii	1e-03	Levenberg-Marquardt nonlinear least squares			
epsilon 1	1.00e-15	∥ J^T e ∥_in f	1e-15	algolithins by M.I.A. Lourakis			
epsilon 2	1.30e-15	Dp _2	1e-15	? levmar link			
epsilon 3	1.00e-30	∥ e ∥_2	1e-20				
delta	delta 1.00e-06 approximation step * 1e-06 Make default						
* delta differe If delta<0, the are more accur employed by de	* delta - difference approximation step, used only in the Bounds mode If delta<0, the Jacobian is approximated with central differences which are more accurate [but stowert] compared to the forward differences employed by default.						











/* Osborne's problem, minimum at (0.3754, 1.9358, -1.4647, 0.0129, 0.0221) */



With Boxes is slower!!



Levmar's examples (#4) : Excel vs. Levmar





Levmar chi-square result by 3 orders of magnitude is lower, than Excel's result!!!



Matrix elements and Beam sigmas plot



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Fitting information window (coming from log-file)



🖶 t4.fit		_	
Initial +641.499	and Final +641.173 LISE fit reduced values		
Parameters: #01: Q084-7TA #02: Q086-7TB #03: Q088-7TC #04: Q098-8TA #05: Q100-8TB #06: Q102-8TC	LeftBound Initial RightBound Final -1.000e+99 < +9.403e+00 < +1.000e+99 +8.916e -1.000e+99 < -1.083e+01 < +1.000e+99 -9.624e -1.000e+99 < +8.752e+00 < +1.000e+99 +7.892e -2.000e+01 < +7.085e+00 < +2.000e+01 +6.310e -4.000e+01 < -5.000e+00 < +2.000e+01 -6.152e -1.000e+01 < +4.212e+00 < +4.000e+01 +3.994e	+00 +00 +00 +00 +00 +00	
Fitting values: #01: sigY #02: sigY #03: sigY #04: sigY #05: focusX #06: focusY #07: X-dispers #08: T-dispers	Initial Final Precision (Fin-Des) +2.469e+01 +1.648e+00 1.000e+00 0.000e+0 +3.323e+01 +3.167e+00 1.000e+00 0.000e+0 +4.555e+01 +6.177e+00 1.000e+00 0.000e+0 +4.716e+01 +7.588e+00 1.000e+00 0.000e+0 +6.022e-01 -1.913e-06 1.000e-03 1.913e-0 -5.364e+00 -8.493e-01 5.000e-01 1.699e+0 -1.287e-13 -1.767e-06 1.000e-02 2.038e-05	<pre>/P Desired 0 < +5.00e+01 0 < +5.00e+01 0 < +5.00e+01 0 < +5.00e+01 3 = +0.00e+00 3 = +0.00e+00 3 = +0.00e+00</pre>	Appears automatically after fitting process completed
#09: sigmaX #10: sigmaY	+3.618e+00 +1.991e+00 1.000e-01 9.911e-0 +6.510e+01 +1.134e+01 1.000e-02 1.035e+0	1 < +2.00e+00 3 < +1.00e+00	It is planning to use different colors and fonts to underline, to select key moments
==> Results for t4 Levenberg-Marquardt Solution: 8.916349	.fit: returned 500 in 500 iter, reason 3 -9.623625 7.891567 6.309539 -6.152035 3.993	751	
<pre>Hinimization info: 0: 4.147e+07 1: 4.111e+07 2: 2.840e+00 3: 2.275e-06 4: 2.378e-04 5: 500 6: 3 7: 4499 8: 500 9: 500</pre>	<pre> e _2 at initial p e _2 J^T e _inf Dp _2 mu/max[J^T J]_ii # iterations reason for terminating # function evaluations # Jacobian evaluations # linear systems solved, i.e. # attempts for re</pre>	ducing error	
Termination reason:	3 - stopped by itmax	==> "sigmaY" : .	last fitting block global optical matrix and sigma vector
		+1.991e+00 -1.482e+00 0 -1.428e-03 0	Format [mm-mrad] -1.913e-06 0 0 -1.767e-06 1.99e+00 +5.025e-01 0 0 0 -2.038e-05 3.36e+00 0 -9.083e+00 -8.493e-01 0 1.13e+01 0 0 -3.325e+00 -4.210e-01 0 4.73e+00 4.73e+00 +5.792e-04 0 0 1.0 -1.088e+01 7.62e-01
		Covariance of t +3.071318e+15 - -7.383595e+15 + +5.433800e+15 - +7.835533e+16 - -1.408364e+17 + +4.149371e+16 -	he fit : 7.383656e+15 +5.433857e+15 +6.802513e+16 -1.067550e+17 +2.799623e+15 1.775066e+16 -1.306325e+16 -1.635389e+17 +2.566550e+17 -6.742622e+15 1.306322e+16 +9.613624e+15 +1.203536e+17 -1.888818e+17 +4.964434e+15 1.883748e+17 +1.386313e+17 +1.182920e+18 -9.006090e+17 -1.998218e+18 3.385910e+17 -2.491815e+17 -1.296397e+18 -1.118888e+18 +6.699783e+18 9.976589e+16 +7.342309e+16 -1.150617e+18 +5.385893e+18 -7.714485e+18



Example for A1900 (1)







Example for A1900 (1)



+4.103e+00

¢10: sigmaY

+8.802e+01

+3.395e+00

The last constaint was not succesfull

The Quad field value was not restored exactly

+4.212e+00

+4.000e+01

-1.000e+01

G

₩UБ: QIUZ—8IC

17

Desired

< +1.00e+00

2.405e+02

1.000e-02

Example for A1900 (2) -- only last triplet to use in fit



19: sigmaX

#10: sigmaY

+4.744e+00

+8.802e+01

The Quad field value was restored

G

All constraints are good!

1.000e-01 1.000e-02

+2.414e+00

+4.777e-01

5.564e-01

5.931e-01

< +3.00e+00

< +1.00e+00

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to

Drs. M.Hausmann, M.Portilio, and D.Weisshaar (NSCL/MSU), for fruitful discussions.