

Optimization software for medium and large-scale problems



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Outline

- MATLAB Optimization Toolbox
- Problem types and algorithms
- Optimization settings
- Function handles and GUI
- cvx
- Other optimization tools in MATLAB
- GAMS
- Online resources

MATLAB Optimization Toolbox

- Widely used algorithms for standard and large-scale optimization
- Constrained and unconstrained problems
- Continuous and discrete variables
- Variety of problems:
 - Linear programming (LP)
 - Quadratic programming (QP)
 - Binary integer programming
 - (General) Nonlinear optimization
 - Multi-objective optimization
- Key features:
 - Find optimal solutions
 - Perform tradeoff analysis
 - Balance multiple design alternatives
 - Support for parallel computing.

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Algorithms for specific types of problems

- Continuous variables

- Constrained, convex

- Linear program: `linprog`
 - Quadratic program: `quadprog`

- Nonlinear

- Unconstrained: `fminunc` (local minimum of multivariate function), `fminsearch`
 - Constrained: `fmincon`, `fminbnd` (single variable bounded minimization), `fseminf` (semi-infinite constraints)
 - Example of `fseminf`: minimize $(x - 1)^2$, subject to $0 \leq x \leq 2$ and $g(x, t) = (x - 0.5) - (t - 0.5)^2 \leq 0, \forall t \in [0, 1]$.

- Least squares

- Linear objective, constrained: `lsqnonneg`, `lsqlin`
 - Nonlinear objective: `lsqnonlin`, `lsqcurvefit`

- Multi-objective: `fgoalattain`, `fminimax`

- Discrete variables

- Binary integer programming: `bintprog`
 - Minimize $f(x)$ subject to $Ax = b, Cx \leq d$
 - $x \in \{0, 1\}^n$.

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 - $\mathbf{x} \in \{0, 1\}^n$.

Optimization problem syntax

Example LP:

minimize $\mathbf{c}^T \mathbf{x}$
subject to $\mathbf{A}\mathbf{x} \leq \mathbf{b}$
 $\mathbf{C}\mathbf{x} = \mathbf{d}$
 $\mathbf{l} \leq \mathbf{x} \leq \mathbf{u}$

MATLAB syntax:

```
[x,fval,exitflag,output,lambda]  
= linprog(c,A,b,C,d,l,u,...  
x0,options)
```

- x_0 : initial value for \mathbf{x}
- `exitflag`: reason for algorithm termination; useful for debugging
- `lambda`: Lagrangian multipliers
- `output`: Number of iterations, algorithm used, etc.

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Choosing an algorithm

- Large-scale

- Uses linear algebra that does not need to store, or operate on, full matrices
- Preserves sparsity structure

- Medium-scale

- Internally creates full matrices
- Requires lot of memory
- Time-intensive computations.

Unconstrained nonlinear algorithms

- `fminunc`
 - Large-scale: user-supplied Hessian, or finite difference approximation
 - Medium-scale: cubic line search; uses quasi-Newton updates of Hessian
- `fminsearch`
 - Derivative-free method (Nelder-Mead simplex)
- `fsolve`
 - Trust-region-dogleg: specially designed for nonlinear equations
 - Trust-region reflective: effective for large-scale (sparse) problems
 - Levenberg-Marquardt

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Constrained linear and nonlinear algorithms

- **fmincon**
 - Trust-region reflective: subspace trust-region method; user-specified gradient; special techniques like Hessian multiply; large-scale
 - Active set: sequential quadratic programming method; medium-scale method; large step size (faster)
 - Interior point: log-barrier penalty term for inequality constraints; problem reduced to having only equality constraints; large-scale
- **linprog**
 - Large-scale interior point
 - Medium-scale active set
 - Medium-scale simplex
- **quadprog, lsqlin**
 - Large-scale
 - Medium-scale
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linprog demo

A farmer wants to decide how to grow two crops x and y on 75 acres of land in order to maximize his profit $143x + 60y$, subject to a storage constraint $110x + 30y \leq 4000$ and an investment constraint $120x + 210y \leq 15000$.

$$\begin{array}{ll} \text{minimize} & -(143x + 60y) \\ \text{subject to} & x + y \leq 75 \\ & 110x + 30y \leq 4000 \\ & 120x + 210y \leq 15000 \\ & -x \leq 0 \\ & -y \leq 0. \end{array}$$

quadprog demo 1

Support vector machine (SVM):

Given the set of labeled points $\{\mathbf{x}_i, y_i\}_{i=1}^m$, $y_i \in \{-1, +1\}$, which is linearly separable, find the vector \mathbf{w} which defines the hyperplane separating the set with maximum margin, i.e.,

$$\begin{aligned}\mathbf{x}_i^T \mathbf{w} - b &\geq 1, \text{ if } y_i = 1 \\ \mathbf{x}_i^T \mathbf{w} - b &\leq -1, \text{ if } y_i = -1.\end{aligned}$$

$$\mathbf{A} := \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_m^T \end{bmatrix}, \mathbf{D} = \text{diag}(y_1, \dots, y_m) \Rightarrow \mathbf{D}(\mathbf{A}\mathbf{w} - \mathbf{b}) \geq \mathbf{1}$$

$$\begin{aligned}\text{minimize} & \quad \|\mathbf{w}\|_2^2 \\ \text{subject to} & \quad \mathbf{D}(\mathbf{A}\mathbf{w} - \mathbf{b}) \geq \mathbf{1}.\end{aligned}$$

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quadprog demo 2

$$\begin{array}{ll} \text{minimize} & 4x_1^2 + x_1x_2 + 4x_2^2 + 3x_1 - 4x_2 \\ \text{subject to} & x_1 + x_2 \leq 5 \\ & -x_1 \leq 0 \\ & -x_2 \leq 0 \\ & x_1 - x_2 = 0. \end{array}$$

$$f(x_1, x_2) = \frac{1}{2}[x_1 \ x_2]^T \begin{bmatrix} 8 & 1 \\ 1 & 8 \end{bmatrix} [x_1 \ x_2] + [3 \ -4]^T [x_1 \ x_2].$$

Function handles and GUI

- A standard MATLAB data type that provides a means of calling a function indirectly: `handle = @functionname`
- Widely used in optimization
- MATLAB GUI for optimization: `optimtool`.

fmincon demo

Rosenbrock function:

$$\begin{aligned} & \text{minimize} && 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \\ & \text{subject to} && x_1^2 + x_2^2 \leq 1. \end{aligned}$$

Choose $[0, 0]^T$ as the initial point.

- MATLAB-based modeling system for *disciplined convex programming*
- Supports the formulation and construction of **convex** optimization problems (convexity to be ensured by user)
- Features:
 - SeDuMi and SDPT3 interior-point solvers
 - Well-defined problems (LP, SOCP, SDP) handled exactly
 - Supports functions that are (good) approximations of convex problems, or can be obtained from successive convex approximations.

¹Developed by Michael Grant and Stephen Boyd, Stanford

Quadratic program:

$$\begin{aligned} & \text{minimize} && 4x_1^2 + x_1x_2 + 4x_2^2 + 3x_1 - 4x_2 \\ & \text{subject to} && x_1 + x_2 \leq 5 \\ & && -x_1 \leq 0 \\ & && -x_2 \leq 0 \\ & && x_1 - x_2 = 0. \end{aligned}$$

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Other optimization tools in MATLAB

- Genetic algorithms and direct search toolbox
 - Derivative-free methods
 - Pattern search
 - Simulated annealing
- Global optimization toolbox
 - Global solutions to problems with multiple extrema
 - General objective and constraint functions:
 - continuous/discontinuous
 - stochastic
 - may include simulations or black-box functions
 - may not possess derivatives.

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TOMLAB

- General-purpose development and modeling environment for optimization problems
- Compatible with MATLAB Optimization Toolbox
- MATLAB solver algorithms, as well as state-of-the-art optimization software packages

Key features:

- Faster and more robust compared to built-in MATLAB solvers
- Automatic, efficient differentiation
- Robust solution of **ill-conditioned nonlinear least squares problems** with linear constraints using several different solver options
- Special treatment of **exponential fitting** and other types of **nonlinear parameter estimation** problems.

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GAMS

- General Algebraic Modeling System
- User-friendly syntax
- Suitable for large-scale problems
- Different types of solvers:
 - Linear programs
 - Mixed integer programs
 - Nonlinear programs
 - Constrained nonlinear systems
 - Quadratically constrained programs
 - Mixed complementarity problems
- Facilitates sensitivity analysis

Illustrative example: Linear program

- **Indices:** i = plants, j = markets
- **Given data:**
 - a_i = supply of commodity at plant i
 - b_j = demand for commodity at market j
 - c_{ij} = cost per unit shipment between plant i and market j
- **Decision variable:** x_{ij} = amount of commodity to ship from plant i to market j
- **Constraints:**
 - $x_{ij} \geq 0$
 - Observe supply limit at plant i : $\sum_j x_{ij} \leq a_i \forall i$
 - Satisfy demand at market j : $\sum_i x_{ij} \geq b_j \forall j$
- **Objective function:** minimize $\sum_{i,j} c_{ij} x_{ij}$

Modeling in GAMS

Good modeling practices:

- Model entities identified and grouped by type
- No symbol referred to before it is defined

Terminology:

- Indices \rightarrow sets
- Given data \rightarrow parameters
- Decision variables \rightarrow variables
- Constraints and objective functions \rightarrow equations

GAMS demo

	Shipping distance ($\times 1000$ miles)			Supplies
	Markets			
Plants	New York	Chicago	Topeka	
Seattle	2.5	1.7	1.8	350
San Diego	2.5	1.8	1.4	600
Demand	325	300	275	

Unit shipping cost: \$90

Structure of a GAMS model

Inputs	Outputs
Sets Declaration Assignment of members	Echo print Reference maps Equation listings Status reports
Data (Parameters, Tables, Scalar) Declaration, assignment of values	Results
Variables Declaration - assignment of type	
Bounds, initial values (optional)	
Equations Declaration, definition	
Model and Solve	

GAMS: Advantages

- Algebra-based notation: easy-to-read for both user and computer
- Reusability of GAMS models
- Model documentation
- Output report easy to interpret
- Extensive debugging ability of compiler
- Models scalable for large problems

Penn State computing resources

- High Performance Computing (HPC) group
- Develops and maintains state-of-the-art computational clusters
- Separate clusters for interactive and batch programming
- Support and expertise for research using programming languages, numerical libraries, statistical packages, finite element solvers, and specialized software
- Expertise for code optimization and parallelization on high performance computing machines
- University-wide access to variety of licensed computational software
- Seminars on data-intensive and numerically-intensive computing

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Online resources

- MATLAB Optimization Toolbox [documentation](#)
- Detailed [listing](#) of optimset options
- cvx [user guide](#)
- NEOS Optimization software guide
- TOMLAB [documentation](#)
- GAMS [documentation](#)