

Lecture 4
Scientific Computing:
Optimization Toolbox
Nonlinear Equations, Numerical Optimization

Matthew J. Zahr

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Advanced MATLAB for Scientific Computing
Stanford University

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Announcement

- Lecture 4 of 8 (or 9)
 - Numerical Optimization (Optimization Toolbox)
- Homework 1 due today
 - I'll grade them on Friday
- Homework 2 posted (only need to do 1 out of 4)
- Need to start thinking about topics for Lecture 9



- 1 Definitions
- 2 Nonlinear System of Equations
- 3 Numerical Optimization
 - Optimization Solvers
 - Optimization Problems
 - Optimization Toolbox



Outline

- 1 Definitions
- 2 Nonlinear System of Equations
- 3 Numerical Optimization
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Scalar-valued function derivatives

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a sufficiently smooth function of n variables.

- Jacobian of f :

$$\frac{\partial f}{\partial \mathbf{x}}(\mathbf{x}) = \left[\frac{\partial f}{\partial x_1}(\mathbf{x}) \quad \cdots \quad \frac{\partial f}{\partial x_n}(\mathbf{x}) \right]$$

- Gradient of f :

$$\nabla f(\mathbf{x}) = \frac{\partial f}{\partial \mathbf{x}}(\mathbf{x})^T = \left[\frac{\partial f}{\partial x_1}(\mathbf{x}) \quad \cdots \quad \frac{\partial f}{\partial x_n}(\mathbf{x}) \right]^T$$

- Hessian of f :

$$[\nabla^2 f(\mathbf{x})]_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{x})$$



Vector-valued function derivatives

Let $\mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a sufficiently smooth function of n variables.

- Jacobian of \mathbf{F} :

$$\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}(\mathbf{x}) \right]_{ij} = \frac{\partial \mathbf{F}_i}{\partial x_j}(\mathbf{x})$$

- Gradient of \mathbf{F} :

$$\nabla \mathbf{F}(\mathbf{x}) = \left(\frac{\partial \mathbf{F}}{\partial \mathbf{x}}(\mathbf{x}) \right)^T$$

- Hessian of \mathbf{F} :

$$[\nabla^2 \mathbf{F}(\mathbf{x})]_{ijk} = \frac{\partial^2 \mathbf{F}_i}{\partial x_j \partial x_k}(\mathbf{x})$$



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Problem Definition

Find $\mathbf{x} \in \mathbb{R}^n$ such that

$$\mathbf{F}(\mathbf{x}) = \mathbf{0} \quad (1)$$

where $\mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ continuously differentiable, nonlinear function.

- Solution methods for (1) iterative, in general
 - Require initial guess and convergence criteria
- Solution for (1) not guaranteed to exist
- If solution of (1) exists, not necessarily unique
 - The solution found depends heavily on the initial guess



Example

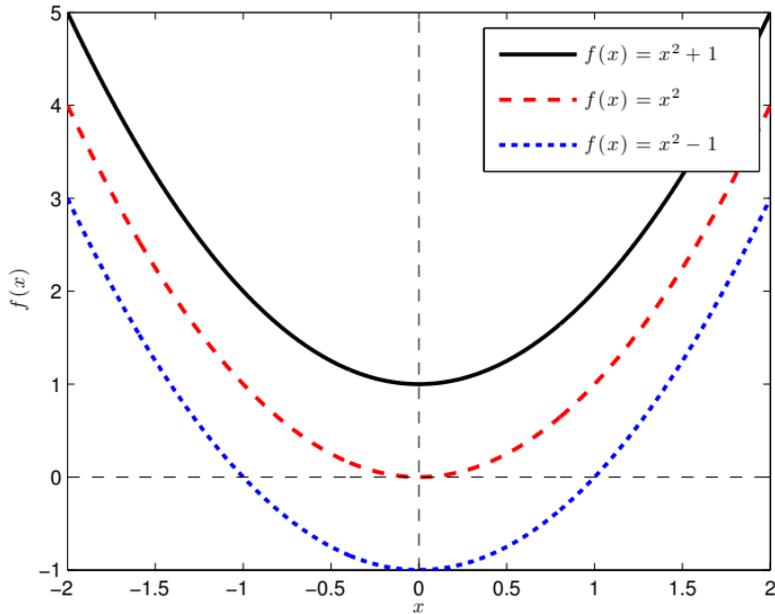


Figure : Non-existence and non-uniqueness of nonlinear equations



Scalar-Valued, Univariate Nonlinear Equation

- Equation (1) with $m = n = 1$ reduces to $f(x) = 0$
- Solution methods
 - Derivative-free methods
 - Only require evaluations of $f(x)$
 - Bisection, Fixed point iteration, etc
 - Demo: `bisection_demo.m`
 - Gradient-based methods
 - Requires function, $f(x)$, and gradient, $f'(x)$, evaluations
 - **Newton's method**
 - Secant method: use finite differences to approximate gradients instead of analytic gradients (only requires function evaluations)
- `fzero`
 - Derivative-free
 - Combines bisection, secant, and interpolation methods



Newton's Method

- Iterative method to solve $f(x) = 0$
- Expand $f(x)$ in a truncated Taylor series about current iteration

$$f(x) = f(x_k) + f'(x_k)(x - x_k) + \mathcal{O}((x - x_k)^2) = 0$$

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

- Demo: `newton_demo.m`



MATLAB builtin command for finding a root of a continuous, scalar-valued, univariate function

- `[x, fval, exitflag, output] = fzero(fun, x0, options)`
 - Inputs
 - `fun` - function handle containing scalar-valued function
 - `x0` - initial guess for root
 - `options` - structure containing options
 - Outputs
 - `x` - root found
 - `fval` - value of `fun` at `x`
 - `exitflag` - convergence flag
 - `output` - structure containing information about solver



Assignment

- Use `fzero` to solve $f(x) = x^2 - 1$
 - Start from any point away from ± 1
- Use `fzero` to solve $f(x) = x^2$
 - Start from any point away from 0
- Use `fzero` to solve $f(x) = x^2 + 1$
 - Start from any point away from 0



Vector-Valued, Multivariate Nonlinear Equations

- Solution methods for (1) in general case
 - Derivative-free methods
 - Requires function, $\mathbf{F}(\mathbf{x})$, evaluations
 - Fixed point iteration, Secant method, etc
 - Gradient-based methods
 - Requires function, $\mathbf{F}(\mathbf{x})$, and Jacobian, $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}(\mathbf{x})$, evaluations
 - **Newton-Raphson method**
 - Gauss-Newton and Levenberg-Marquardt (nonlinear least squares: $\min \|\mathbf{F}(\mathbf{x})\|$)
 - Can use finite difference approximations to gradients instead of analytic gradients (only requires function evaluations)
- `fsolve`
 - Gradient-based



MATLAB builtin command for finding a root of a continuous, vector-valued, multivariate function

- `[x, fval, exitflag, output, jac] = fzero(fun, x0, options)`
 - Inputs/Outputs - same as `fzero`
 - `fun` - function handle containing *vector*-valued function
- Algorithms
 - Standard trust region (default)
 - Requires square system $m = n$
 - Trust region reflexive, Gauss-Newton, Levenberg-Marquardt
 - Nonlinear least squares (use if f may not have root)
- By default uses finite differences to compute Jacobian
- To supply analytic Jacobian
 - `fun` return Jacobian as *second* output
 - `options.Jacobian = 'on'`



Example

- Derive *Jacobian* of

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1 - 4x_1^2 - x_1x_2 \\ 2x_2 - x_2^2 - 3x_1x_2 \end{bmatrix}$$

- Solve $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ using `fsolve`
 - First *without* using Jacobian information
 - Then *with* Jacobian information
(`options = optimset('Jacobian','on')`)
- How do the number of function/Jacobian evaluations compare in the two cases?
 - `output.funcCount`



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Problem Definition

Consider the *general* optimization problem

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && f(\mathbf{x}) \\ & \text{subject to} && \mathbf{A}\mathbf{x} \leq \mathbf{b} \\ & && \mathbf{A}_{eq}\mathbf{x} = \mathbf{b}_{eq} \\ & && \mathbf{c}(\mathbf{x}) \leq \mathbf{0} \\ & && \mathbf{c}_{eq}(\mathbf{x}) = \mathbf{0} \\ & && \boldsymbol{\ell} \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{2}$$

- $\boldsymbol{\ell}, \mathbf{u} \in \mathbb{R}^{n_v}$ are box constraints
- $\mathbf{c} : \mathbb{R}^{n_v} \rightarrow \mathbb{R}^{n_{ineq}^{nl}}$ are nonlinear inequality constraints
- $\mathbf{c}_{eq} : \mathbb{R}^{n_v} \rightarrow \mathbb{R}^{n_{eq}^{nl}}$ are nonlinear equality constraints
- $\mathbf{A} \in \mathbb{R}^{n_{ineq}^{lin} \times n_v}$ define linear inequality constraints
- $\mathbf{A}_{eq} \in \mathbb{R}^{n_{eq}^{lin} \times n_v}$ define linear equality constraints



Feasible Set

For (2), $\mathbf{x} \in \mathbb{R}^{n_v}$ is *feasible* if \mathbf{x} satisfies the constraints

$$\begin{aligned} \mathbf{A}\mathbf{x} &\leq \mathbf{b} \\ \mathbf{A}_{eq}\mathbf{x} &= \mathbf{b}_{eq} \\ \mathbf{c}(\mathbf{x}) &\leq \mathbf{0} \\ \mathbf{c}_{eq}(\mathbf{x}) &= \mathbf{0} \\ \ell &\leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{3}$$

- Define the *feasible set*, $\mathcal{F} = \{\mathbf{x} \in \mathbb{R}^{n_v} \mid \mathbf{x} \text{ satisfies (3)}\}$
- \mathbf{x} is feasible if $\mathbf{x} \in \mathcal{F}$
- If there is no \mathbf{x} such that (3) is satisfied, $\mathcal{F} = \emptyset$ and the problem is said to be *infeasible*
- If $f(\mathbf{x})$ is independent of \mathbf{x} , (2) is said to be a *feasibility* problem



Lagrangian

Write (2) concisely as

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && f(\mathbf{x}) \\ & \text{subject to} && \mathbf{g}(\mathbf{x}) \geq 0 \\ & && \mathbf{h}(\mathbf{x}) = 0 \end{aligned} \tag{4}$$

Define the Lagrangian of (4) as

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\mathbf{x}) - \boldsymbol{\lambda}^T \mathbf{g}(\mathbf{x}) - \boldsymbol{\mu}^T \mathbf{h}(\mathbf{x}) \tag{5}$$

where $\boldsymbol{\lambda}$ are the Lagrange multipliers for the inequality constraints and $\boldsymbol{\mu}$ are the Lagrange multipliers for the equality constraints.

- Notice there is a Lagrange multiplier *for each constraint*, whether the constraint is a simple bound, general linear, nonlinear, equality, or inequality.



Optimality Conditions

- First-order necessary condition
 - Suppose \mathbf{x}^* is a local solution to (4) plus additional assumptions. Then there are Lagrange multipliers, $\boldsymbol{\lambda}^*$ and $\boldsymbol{\mu}^*$, such that the following *Karush-Kuhn-Tucker* (KKT) conditions are satisfied

$$\begin{aligned}\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) &= 0 \\ \mathbf{g}(\mathbf{x}^*) &\geq 0 \\ \mathbf{h}(\mathbf{x}^*) &= 0 \\ \boldsymbol{\mu}^* &\geq 0 \\ \boldsymbol{\lambda}^{*T}\mathbf{g}(\mathbf{x}^*) + \boldsymbol{\mu}^{*T}\mathbf{h}(\mathbf{x}^*) &= 0\end{aligned}\tag{6}$$

- Second-order necessary condition: $\nabla_{\mathbf{xx}}^2\mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) \succeq 0$
- Second-order sufficient condition: $\nabla_{\mathbf{xx}}^2\mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*) \succ 0$



Types of Optimization Solvers: Function Information

- Derivative-free
 - Only function evaluations used
 - Brute force
 - Genetic algorithms
 - Finite difference computations of gradients/Hessians
 - Usually require *very large* number of function evaluations
- Gradient-based
 - Most popular class of techniques
 - Function and gradient evaluations used
 - Finite difference computations of Hessians
 - SPD updates to build Hessian approximations (BFGS)
- Hessian-based
 - Hessians usually difficult/expensive to compute, although often very sparse
 - Second-order optimality conditions
 - Function, gradient, and Hessian evaluations used



Types of Optimization Solvers

- Interior point methods
 - Iterates always strictly feasible
 - Use barrier functions to keep iterates away from boundaries
 - Sequence of optimization problems
- Active set methods
 - Active set refers to the inequality constraints *active* at the solution
 - Possibly infeasible iterates when constraints nonlinear
 - Minimize problem for given active set, then update active set based on Lagrange multipliers



Types of Optimization Solvers: Globalization

- Globalization: techniques to make optimization solver *globally convergent* (convergent to some *local* minima from *any* starting point)
 - Trust region methods
 - Determine step length
 - Define model problem whose solution will be the *step direction*
 - Line search methods
 - Determine search direction (Newton, Quasi-Newton, etc)
 - Find step length based on sufficient decrease criteria



Linear Program

Linear program ($\mathbf{f} \in \mathbb{R}^{n_v}$)

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && \mathbf{f}^T \mathbf{x} \\ & \text{subject to} && \mathbf{A} \mathbf{x} \leq \mathbf{b} \\ & && \mathbf{A}_{eq} \mathbf{x} = \mathbf{b}_{eq} \\ & && \ell \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{7}$$

MATLAB solver (`linprog`)

- Medium-scale
 - Simplex method
 - `options = optimset('LargeScale', 'off', 'Simplex', ... 'on')`
- Large-scale
 - Primal-dual interior point method
 - Default



Binary Integer Linear Program

Binary integer linear program ($\mathbf{f} \in \mathbb{R}^{n_v}$)

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && \mathbf{f}^T \mathbf{x} \\ & \text{subject to} && \mathbf{A} \mathbf{x} \leq \mathbf{b} \\ & && \mathbf{A}_{eq} \mathbf{x} = \mathbf{b}_{eq} \\ & && \mathbf{x}_j \in \{0, 1\} \text{ for } j \in \{0, \dots, n_v\} \end{aligned} \tag{8}$$

MATLAB solver (`bintprog`)

- Linear program branch-and-bound
 - Sequence of LP-relaxation problems



Quadratic Program

Quadratic program ($\mathbf{H} \in \mathbb{R}^{n_v \times n_v}$, $\mathbf{f} \in \mathbb{R}^{n_v}$)

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && \frac{1}{2} \mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{f}^T \mathbf{x} \\ & \text{subject to} && \mathbf{A} \mathbf{x} \leq \mathbf{b} \\ & && \mathbf{A}_{eq} \mathbf{x} = \mathbf{b}_{eq} \\ & && \ell \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{9}$$

MATLAB solver (quadprog)

- Medium-scale
 - Active-set method with linear subproblems
- Large-scale
 - Trust region reflexive method
 - Newton-type method
 - Preconditioned CG to solve linear system



Unconstrained Optimization

$$\underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} \quad f(\mathbf{x}) \quad (10)$$

MATLAB solvers

- MATLAB solvers (fminunc, fminsearch)
 - fminsearch
 - Derivative-free
 - Simplex search
 - fminunc
 - Quasi-Newton with linesearch (medium scale)
 - Trust region reflexive (large scale)



Linearly Constrained Optimization

- General

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && f(\mathbf{x}) \\ & \text{subject to} && \mathbf{Ax} \leq \mathbf{b} \\ & && \mathbf{A}_{eq}\mathbf{x} = \mathbf{b}_{eq} \\ & && \ell \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{11}$$

- Bounds only

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{n_v}}{\text{minimize}} && f(\mathbf{x}) \\ & \text{subject to} && \ell \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{12}$$

MATLAB solvers (fminbnd, fmincon)

- fminbnd
 - Single variable optimization
- fmincon
 - Trust region reflexive method
 - Active-set method



Nonlinearly Constrained Optimization

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^{nv}}{\text{minimize}} && f(\mathbf{x}) \\ & \text{subject to} && \mathbf{Ax} \leq \mathbf{b} \\ & && \mathbf{A}_{eq}\mathbf{x} = \mathbf{b}_{eq} \\ & && \mathbf{c}(\mathbf{x}) \leq \mathbf{0} \\ & && \mathbf{c}_{eq}(\mathbf{x}) = \mathbf{0} \\ & && \ell \leq \mathbf{x} \leq \mathbf{u} \end{aligned} \tag{13}$$

- Solvers
 - Trust region reflexive
 - Sequential Quadratic Programming (SQP)
 - Interior Point (IP)



Optimization Toolbox Syntax

- Syntax for call to Optimization Toolbox
 - `[x, fval, exitflag, out, lam, grad, hess] = ...
solver(f, x0, A, b, Aeq, beq, lb, ub, nlcon, opt)`
 - `[x, fval, exitflag, out, lam, grad, hess] = solver(problem)`
- Outputs
 - `x` - minimum found
 - `fval` - value of objective function at `x`
 - `exitflag` - describes exit condition of solver
 - `out` - structure containing output information
 - `lam` - structure containing Lagrange multipliers at `x`
 - `grad` - gradient of objective function at `x`
 - `hess` - Hessian of objective function at `x`



Optimization Toolbox Syntax

- Syntax for call to Optimization Toolbox
 - `[x, fval, exitflag, out, lam, grad, hess] = ...
solver(f, x0, A, b, Aeq, beq, lb, ub, nlcon, opt)`
 - `[x, fval, exitflag, out, lam, grad, hess] = solver(problem)`
- Inputs
 - `f` - function handle (or vector for LP) defining objective function (and gradient)
 - `x0` - vector defining initial guess
 - `A, b` - matrix, RHS defining linear inequality constraints
 - `Aeq, beq` - matrix, RHS defining linear equality constraints
 - `lb, ub` - vectors defining lower, upper bounds
 - `nlcon` - function handle defining nonlinear constraints (and Jacobians)
 - `opt` - optimization options structure
 - `problem` - structure containing above information



Problem Structure

Instead of specifying many different inputs in a call to the optimizer, store inputs in problem structure

- problem
 - objective
 - x0
 - Aineq, bineq
 - Aeq, beq
 - lb, ub
 - nonlcon
 - solver
 - options
- Helpful in interacting with optimization GUI



Options Structure

- Each optimization solver has tunable options that can be specified with an options structure
 - `optimset <solver>` to return options available for particular solver, along with default values
 - Gives fine-grained control over optimization solver
 - Objective/Constraint functions
 - Maximum iterations
 - Tolerances
 - Difference intervals
 - Gradient, Hessian computations
 - Preconditioning
 - Scaling
 - Parallelization
 - Output and plotting functions



Optimization Functions

- Linear Programming
 - `linprog`
- Binary Integer Programming
 - `bintprog`
- Quadratic Programming
 - `quadprog`
- Unconstrained Optimization
 - `fminsearch`, `fminunc`
- Constrained Optimization
 - General Nonlinear
 - `fminbnd`, `fmincon`, `ktrlink`
 - TOMLAB (commercial software)
 - Least Squares
 - Linear: `lsqlin`, `lsqnonneg`
 - Nonlinear: `lsqcurvefit`, `lsqnonlin`
- Multiobjective Optimization
 - `fgoalattain`, `fminimax`



Objective Function

- Most optimization solvers require *scalar-valued* objective function
 - Exceptions: `fgoalattain`, `fminimax`, `fsolve`, `lsqcurvefit`, `lsqnonlin`
 - Must take optimization variables, \mathbf{x} , as input
 - Must return value of objective function $f(\mathbf{x})$
 - May return gradient, $\nabla f(\mathbf{x})$, and Hessian, $\nabla^2 f(\mathbf{x})$
 - User-supplied gradient only used if: `optimset('GradObj','on')`
 - User-supplied Hessian only used if: `optimset('Hessian','on')`
- For vector-valued objective functions, $\mathbf{F}(\mathbf{x})$
 - Input syntax identical to scalar-valued case
 - Instead of gradient, return *Jacobian* matrix, $\frac{\partial \mathbf{F}}{\partial \mathbf{x}}$



Nonlinear Constraint Functions

- Nonlinear constraints are of the form $\mathbf{c}(\mathbf{x}) \leq 0$, $\mathbf{c}_{eq}(\mathbf{x}) = 0$
- Nonlinear constraint function must return \mathbf{c} and \mathbf{c}_{eq} , even if they both do not exist (use [])
- Call syntax
 - No derivatives: $[\mathbf{c}, \mathbf{c}_{eq}] = \text{constr_func}(\mathbf{x})$
 - Derivatives: $[\mathbf{c}, \mathbf{c}_{eq}, \text{grad_c}, \text{grad_ceq}] = \text{constr_func}(\mathbf{x})$
 - Derivatives must be in the form of *gradients*: $\text{grad_c}(i,j) = \frac{\partial \mathbf{c}_j}{\partial \mathbf{x}_i}$,
 $\text{grad_ceq}(i,j) = \frac{\partial \mathbf{c}_{eq,j}}{\partial \mathbf{x}_i}$



Assignment

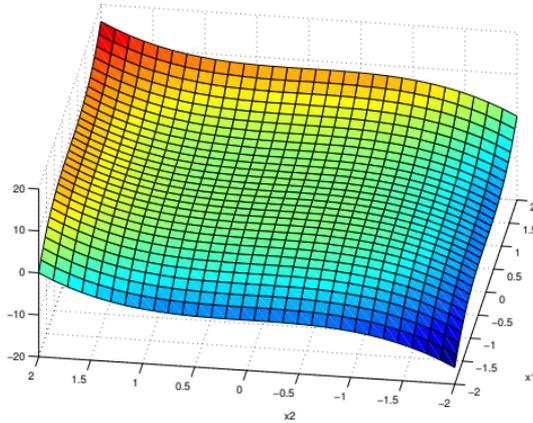
Consider the following *nonlinearly constrained* optimization problem

$$\begin{aligned} & \underset{\mathbf{x} \in \mathbb{R}^2}{\text{minimize}} && \mathbf{x}_1^3 + \mathbf{x}_2^3 \\ & \text{subject to} && \mathbf{x}_1 + 5\mathbf{x}_2 \geq 0 \\ & && \mathbf{x}_1^2 + \mathbf{x}_2^2 \leq 2 \\ & && -2 \leq \mathbf{x} \leq 2 \end{aligned} \tag{14}$$

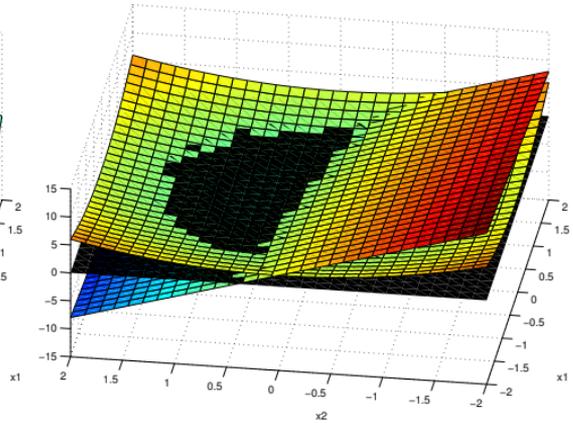
- Derive derivative information for objective and *nonlinear* constraints
- Convert optimization problem into MATLAB compatible form
 - Linear inequality constraints: $\mathbf{Ax} \leq \mathbf{b}$
 - Nonlinear inequality constraints: $\mathbf{c}(\mathbf{x}) \leq \mathbf{0}$
- Solve using `fmincon`



Assignment



(a) Objective Functions



(b) Constraints

Figure : Assignment



Assignment

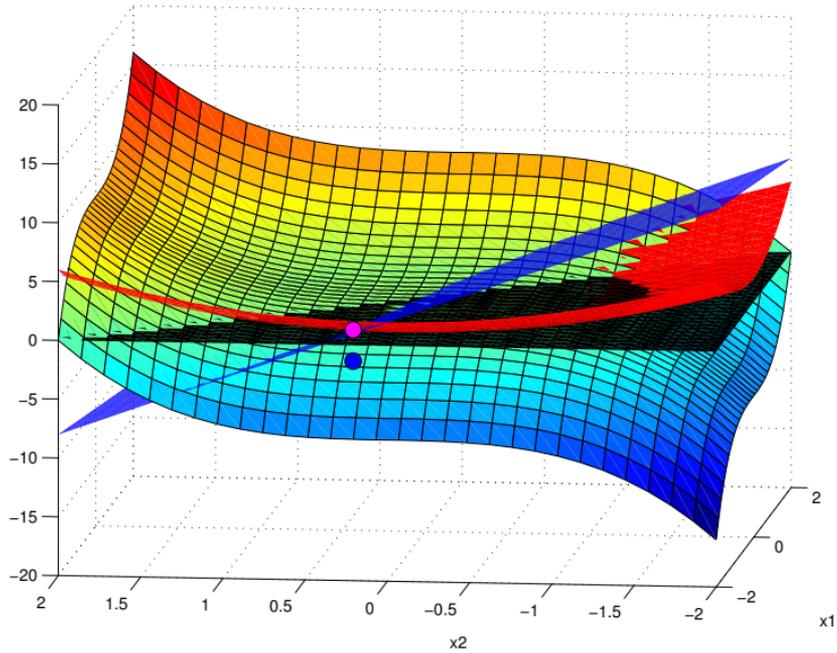


Figure : Assignment with solution



Optimization Toolbox GUI (`optimtool`)

- MATLAB's Optimization Toolbox comes equipped with GUI
 - `optimtool` to launch
 - User-friendly
 - Import problem or options from workspace
 - Generate code
 - Export optimization problem to workspace
- Brief Demo
- Power of MATLAB is scripting capabilities



Large-scale vs. Medium-scale

- *Large-scale* optimization algorithm
 - Linear algebra does not store or operate on *full* matrices
 - Sparse matrices and sparse linear algebra
 - Internal algorithms preserve sparsity or do not generate matrices (iterative solvers)
 - May be used for small problems
- *Medium-scale* optimization algorithms
 - Full matrices and dense linear algebra used
 - May require significant amount of memory and CPU time for large problems
 - Use to access functionality not implemented in *large-scale* case



Choosing an Algorithm

<http://www.mathworks.com/help/optim/ug/choosing-a-solver.html>



Parallel Computing and the Optimization Toolbox

- Parallel Computations available with commands `fmincon`, `fminattain`, `fminimax`
 - Start MATLAB pool of workers
 - Set `UseParallel` option to `'always'`
 - `parfor` to loop over multiple initial conditions
 - Attempt at global optimization
 - Embarrassingly parallel

```
>> matlabpool open 2  
>> options = optimset('UseParallel','always');
```



Passing Additional Arguments to Functions

- An objective function or constraint may require additional arguments besides the optimization variables (\mathbf{x})
- MATLAB's optimizers only pass optimization variables, \mathbf{x} , into functions
- Options for passing additional arguments to functions
 - Store variables in anonymous functions
 - Nested functions (variable sharing between parent/child)
 - Global variables

