

Introduction to (Mathematical) Optimization

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(w/ material from Stephen Boyd and Steven Diamond)

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Optimization

Optimization finding a best (or good enough) choice among the set of options for a certain objective

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- ▶ **system**: mathematical model
- ▶ **change**: change to input variables (parameters)
- ▶ **outcome**: a measure of performance of the model, objective function

Mathematical optimization

Mathematical optimization problem has form

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m\end{array}$$

- ▶ $x \in \mathbf{R}^n$ is **decision variable** (to be found)
- ▶ f_0 is objective function; f_i are constraint functions
- ▶ problem data are hidden inside f_0, \dots, f_m

The good news

Everything is an optimization problem

- ▶ *choose parameters* in model to fit data (minimize misfit or error on observed data)
- ▶ *optimize actions* (minimize cost or maximize profit)
- ▶ *allocate resources* over time (minimize cost, power; maximize utility)
- ▶ *engineering design* (trade off weight, power, speed, performance, lifetime)

The bad news

In full generality, optimization problems can be quite difficult

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- ▶ heuristics required, hand-tuning, luck, babysitting

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But...

- ▶ we can do a lot by restricting to convex models (AJ's talk)
- ▶ we have good computational tools
 - ▶ modeling languages (CVX, CVXPY, JuMP, AMPL, GAMS) to write problems down
 - ▶ solvers (IPOPT, SNOPT, Gurobi, CPLEX, Sedumi, SDPT3, ...) to obtain solutions

Example: The Raptor Problem

See other slides

Optimization in one variable

$$\text{minimize } f(x) \in C^2 : \mathbf{R} \rightarrow \mathbf{R}$$

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- ▶ Local optimization: look for a point x^* such that $f(x^*) \leq f(x)$ for all points x near x^*

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- ▶ Global optimization: look for a point x^* such that $f(x^*) \leq f(x)$ for all points x in domain of interest
- ▶ When $f(x)$ is twice continuously differentiable, then local optimization involves finding a point x^* such that $f'(x^*) = 0$ and $f''(x^*) > 0$

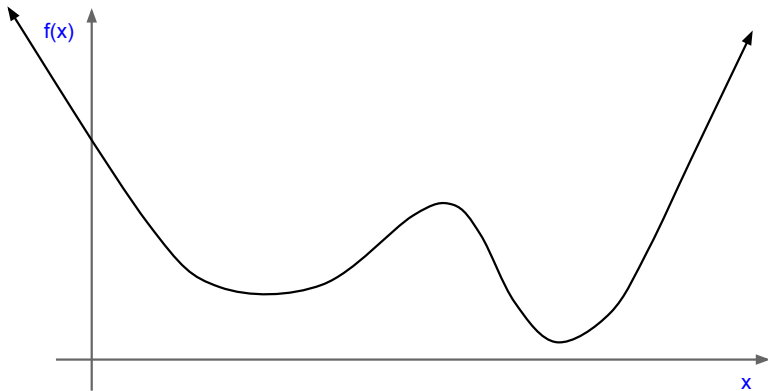
Optimization in one variable: axis



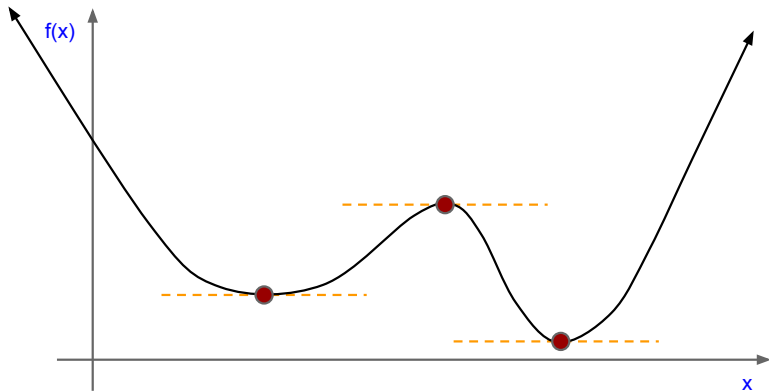
Optimization in one variable: definitions



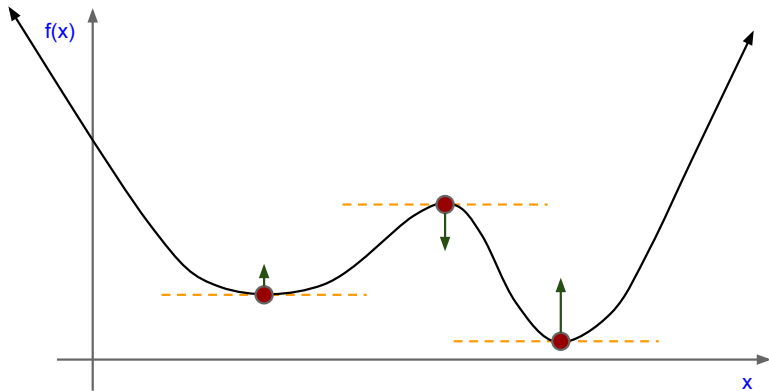
Optimization in one variable: example objective function



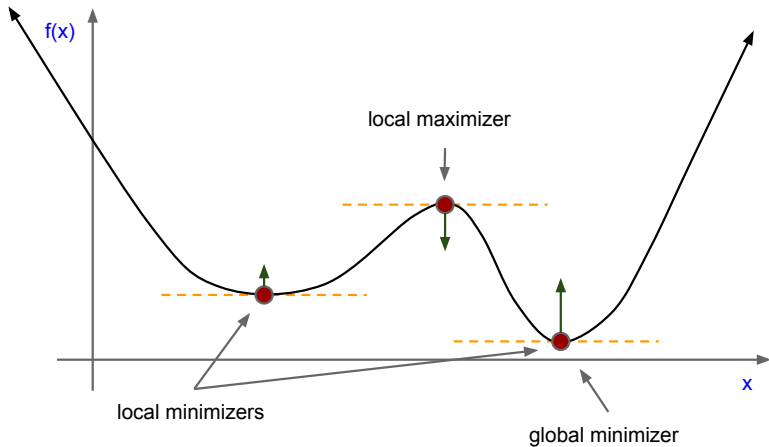
Optimization in one variable: critical points, $f'(x) = 0$



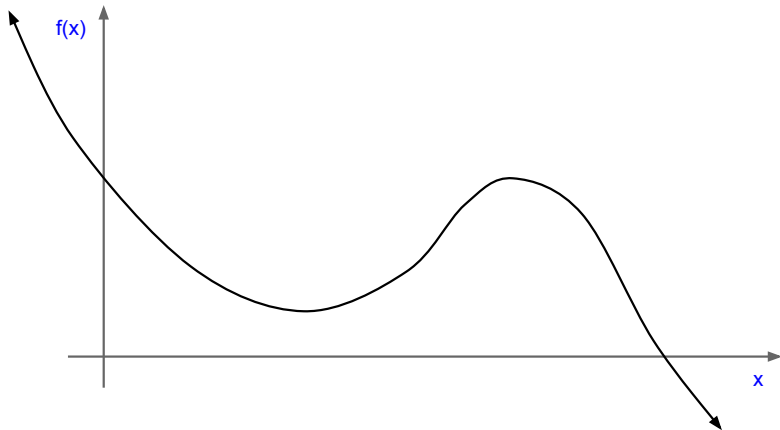
Optimization in one variable: local optima



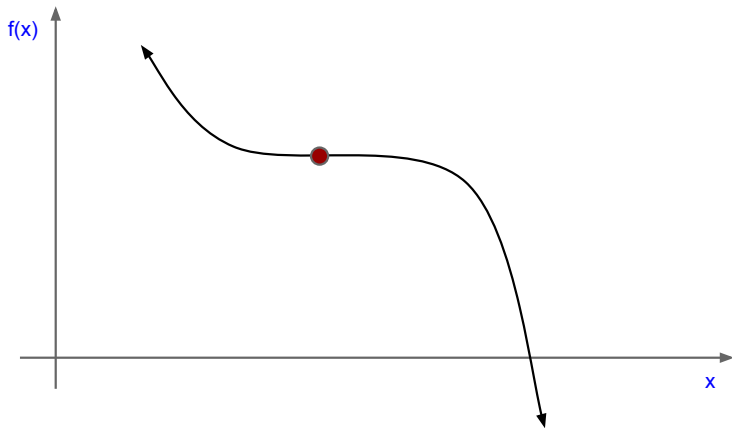
Optimization in one variable: local optima, $f''(x) = ?$



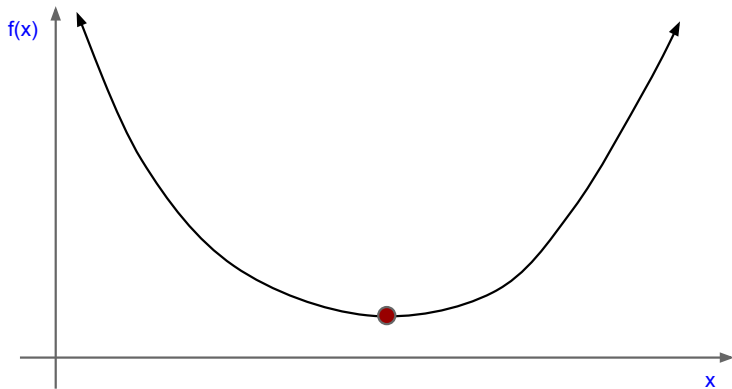
Optimization in one variable: unbounded below



Optimization in one variable: saddle point, $f'(x) = 0$ and $f''(x) = 0$



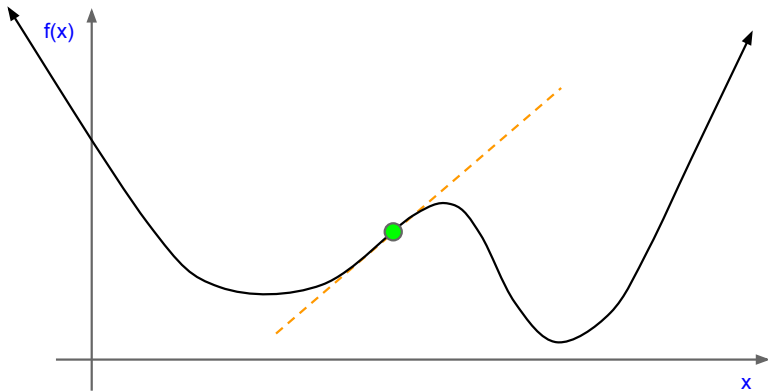
Optimization in one variable: convex objective



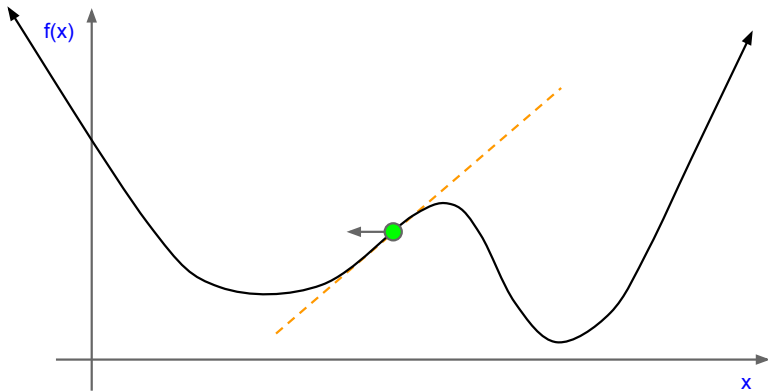
Key definitions

- ▶ *domain*: space for input variable x
- ▶ *range*: space for output of objective function $f(x)$
- ▶ *critical point*: $f'(x) = 0$
- ▶ *local minimizer*: $f'(x) = 0$ and $f''(x) > 0$
- ▶ *local maximizer*: $f'(x) = 0$ and $f''(x) < 0$
- ▶ *saddle point*: $f'(x) = 0$ and $f''(x) = 0$
- ▶ *global minimizer*: x^* such that $f(x^*) \leq f(x)$ for all x in domain

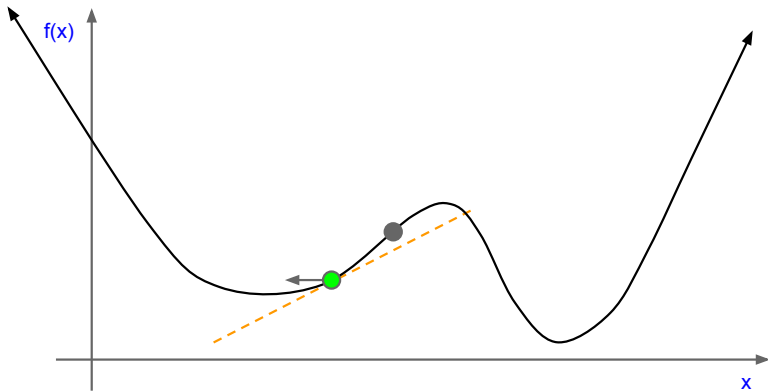
Optimization in one variable: algorithm basics



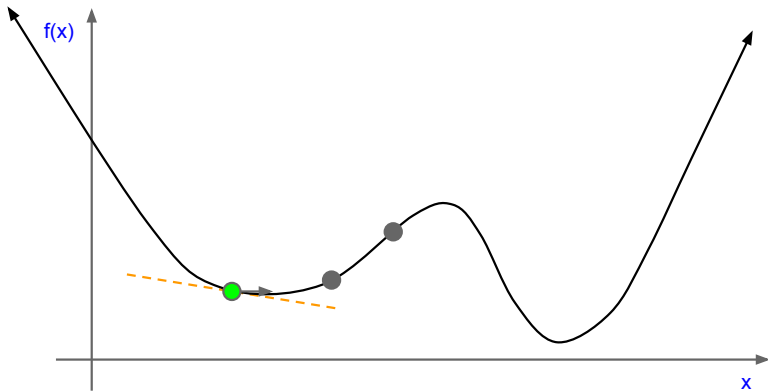
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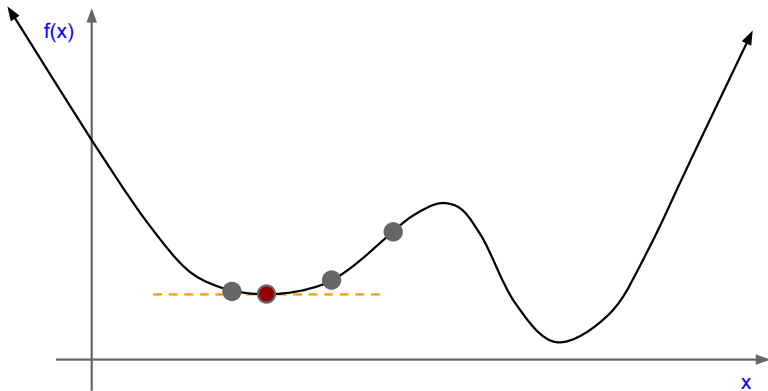
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- ▶ Key algorithm property: ***descent condition***

$$f(x_{k+1}) < f(x_k)$$

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$$f(x_{k+1}) < f(x_k)$$

- ▶ Technical algorithm property: ***convergence to solution***

$$|x_{k+1} - x_k| \rightarrow 0 \text{ if and only if } f'(x_k) \rightarrow 0 \text{ and } \lim_{k \rightarrow \infty} f''(x_k) \geq 0$$

Optimization in many variables

$$\text{minimize } f(x) \in C^2 : \mathbf{R}^n \rightarrow \mathbf{R}$$

- ▶ x is an n -dimensional vector of real variables
- ▶ $f(x)$ is the objective function (twice continuously differentiable)
 - ▶ First derivative or gradient of f is written $\nabla f(x)$
 - ▶ Second derivative or Hessian of f is written $\nabla^2 f(x)$
- ▶ We are looking for a point x^* such that $\nabla f(x) = 0$ and $\nabla^2 f(x) \succeq 0$. Note that this is a *local* optimizer
 - ▶ $\nabla^2 f(x) \succeq 0$ means that all the eigenvalues of $\nabla^2 f(x)$ are non-negative

The gradient $\nabla f(x)$ in 2 variables

Vector of variables:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Gradient of f :

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

The Hessian $\nabla^2 f(x)$ in 2 variables

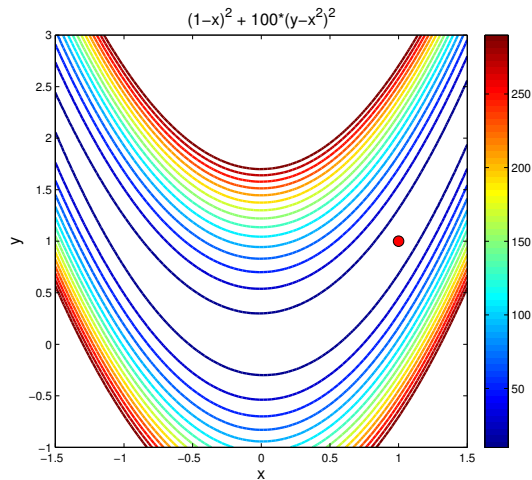
$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

Let's look at an example

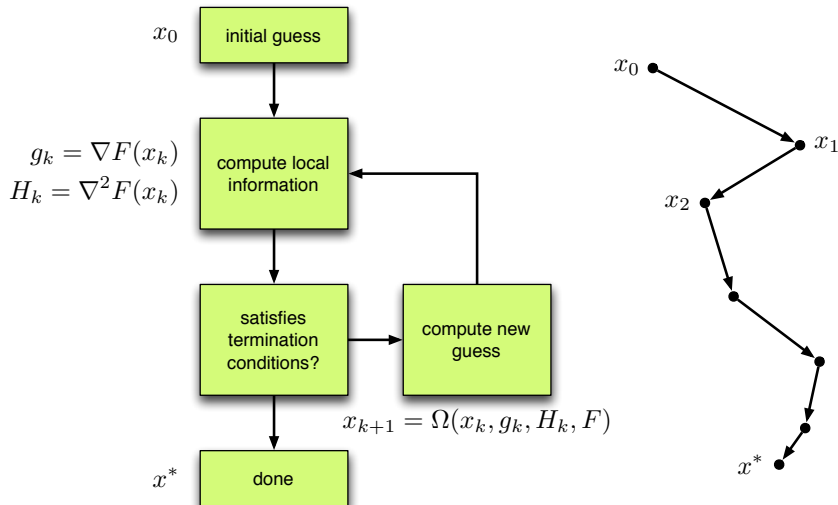
The Rosenbrock function:

$$f(x, y) = (1 - x)^2 + 100 (y - x^2)^2$$

Rosenbrock contours



Basic optimization algorithm



Line search algorithms

1. compute a search direction p_k
 - ▶ for minimization, p_k must be a descent direction, that is $p_k^T g_k < 0$
2. select a step length α_k along p_k such that $f(x_k + \alpha_k p_k) < f(x_k)$
 - ▶ (we need more technical requirements here)
3. update the guess $x_{k+1} \leftarrow x_k + \alpha_k p_k$

Example line search algorithms

Algorithm:

$$x_{k+1} \leftarrow x_k + \alpha_k p_k$$

Gradient descent:

$$p_k = -g_k = -\nabla f(x_k)$$

Modified Newton's method:

$$p_k = -(H_k + \lambda_k I)^{-1} g_k = (\nabla^2 f(x_k) + \lambda_k I)^{-1} \nabla f(x_k)$$

Step length selection: backtracking

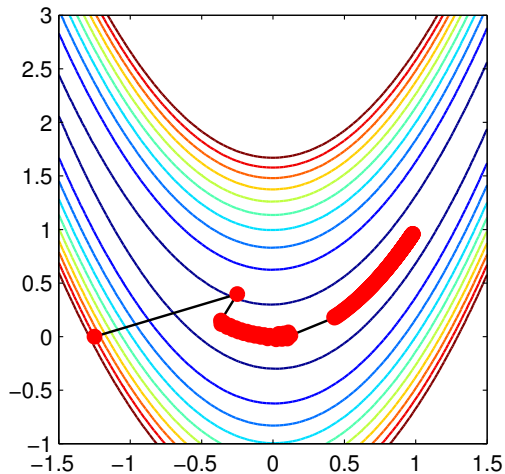
Goal: given p_k find α such that $f(x_k + \alpha p_k) < f(x_k)$.

Procedure: start with initial guess $\alpha > 0$ (use $\alpha = 1$ for Newton's method)

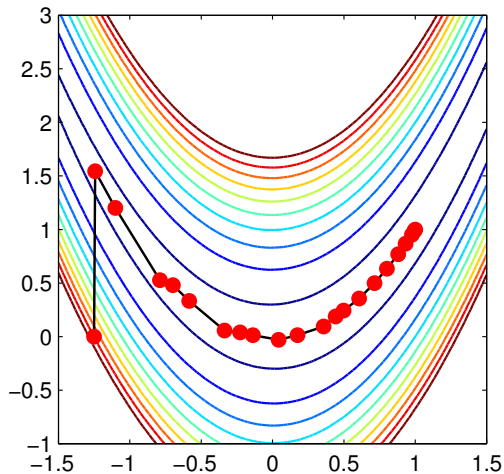
1. if $f(x_k + \alpha p_k) < f(x_k)$, then return α , otherwise continue
2. decrease α by some factor $0 < \delta < 1$: $\alpha \leftarrow \delta \alpha$
3. repeat

Optimization on rosenbrock function

Gradient descent

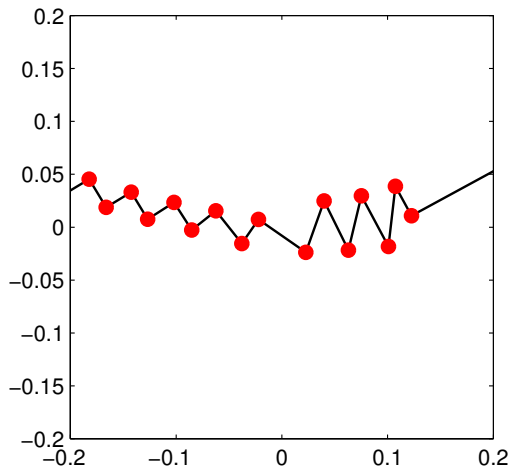


Newton's method

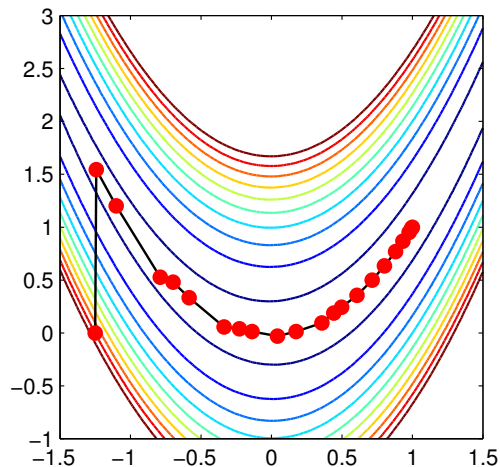


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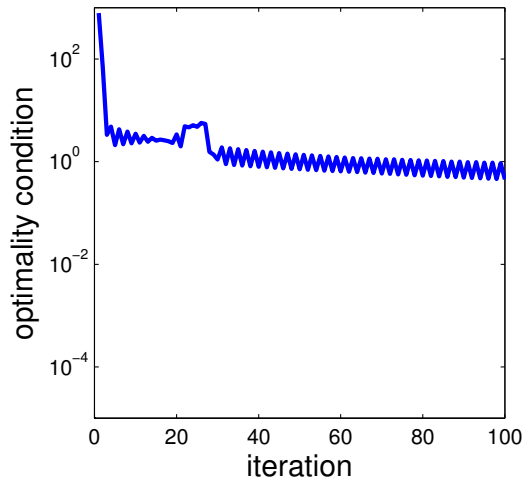


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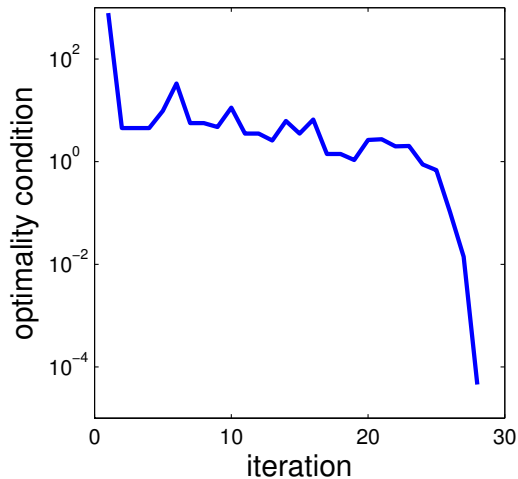


Optimization on rosenbrock function

Gradient descent



Newton's method



Considerations in selecting optimization algorithms

- ▶ Computational cost/scale of objective function
- ▶ Computational cost of linear algebra associated with optimization algorithm
- ▶ Accuracy requirement in your application

Two very important optimization problems

- ▶ linear least squares
- ▶ non-linear least squares

Constraints

- ▶ basic idea of constraints
- ▶ work through example from multivariate calculus
- ▶ introduce idea of multipliers
- ▶ equality constraints
- ▶ inequality constraints
- ▶ linear constraints
- ▶ nonlinear constraints

Penalty and barrier methods

- ▶ introduce a penalty into the objective to penalize constraint violation

Linear programming

Discrete variables

- ▶ Mixed integer programming
- ▶ Scheduling problems

What's next

- ▶ Nonlinear programming
- ▶ Convex modelling
- ▶ Study of algorithms
- ▶ Modeling languages
- ▶ Automated differentiation