

Today

- non lin. h of
- optimization

Announcements

- HW8
- 4CH

Fixed Point Iteration

lin. $|g'(x^*)| < 1$
quad. $g'(x^*) = 0$

When does this converge?

$$x_0 = \langle \text{starting guess} \rangle$$

$$x_{k+1} = g(x_k)$$

$$f: \mathbb{R}^n \rightarrow \mathbb{R}^k$$

$$g: \mathbb{R}^k \rightarrow \mathbb{R}^k$$

inputs

$$\partial g(x) = \begin{pmatrix} \partial_{x_1} g_1 \\ \partial_{x_1} g_2 \end{pmatrix}$$

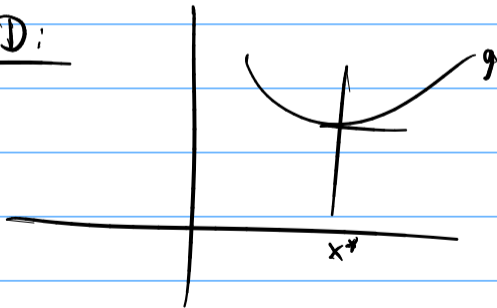
outputs

$$\|\partial g\|_p < 1 \Rightarrow \rho(\partial g(x^*)) < 1 \Rightarrow \text{lin. conv.}$$

$$\nabla g(\vec{x}^*) = 0 \Rightarrow \text{quod. conv.}$$

$$\vec{J} g(\vec{x} + \vec{h}) = \vec{J} g(\vec{x}) + \nabla g(\vec{x}) \cdot \vec{h}$$

In 1D:



$$f_1(x_1, x_2) = 0$$

$$f_2(x_1, x_2) = 0$$

Newton's Method

What does Newton's method look like in n dimensions?

$$\circlearrowleft \Rightarrow f(\vec{x}_n + \vec{h}) = f(\vec{x}_n) + J_f(\vec{x}_n) \cdot \vec{h} + \cancel{O(h^2)}$$

$$- f(\vec{x}_n) - J_f(\vec{x}_n) \cdot \vec{h}$$

$$- J_f(\vec{x}_n)^{-1} f(\vec{x}_n) = \vec{h}$$

$$\vec{x}_{n+1} = \vec{x}_n - J_f^{-1}(\vec{x}_n) \cdot f(\vec{x}_n)$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

nD

$1D$

Downsides of n -dim. Newton?

- local conv.

- $J_f \leftarrow$

Demo: Newton's method in n dimensions

Secant in n dimensions?

$$x_k = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix} \quad x_{k-1} = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix}$$
$$f(x_k) = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix} \quad f(x_{k-1}) = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

What would the secant method look like in n dimensions?

$$\frac{f(x + h\vec{e}_i) - f(x)}{h} \rightarrow \text{first column of } {}^n J_f^n$$

$$\tilde{J}_0 = I \quad \rightsquigarrow \text{with eval of } f(x_1), f(x_0),$$

update \tilde{J}_i

Broyden's method

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

- Methods for unconstrained opt. in one dimension

- Methods for unconstrained opt. in n dimensions

- Nonlinear Least Squares

- Constrained Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Optimization: Problem Statement

Have: Objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$

Want: Minimizer $\mathbf{x}^* \in \mathbb{R}^n$ so that

$$f(\mathbf{x}^*) = \min_{\mathbf{x} \in \mathcal{K}} f(\mathbf{x}) \quad \text{subject to} \quad \mathbf{g}(\mathbf{x}) = \mathbf{0} \quad \text{and} \quad \mathbf{h}(\mathbf{x}) \leq \mathbf{0}.$$

- ▶ $\mathbf{g}(\mathbf{x}) = \mathbf{0}$ and $\mathbf{h}(\mathbf{x}) \leq \mathbf{0}$ are called **constraints**.
They define the set of **feasible points** $\mathbf{x} \in S \subseteq \mathbb{R}^n$.
- ▶ If \mathbf{g} or \mathbf{h} are present, this is **constrained optimization**.
Otherwise **unconstrained optimization**.
- ▶ If f , \mathbf{g} , \mathbf{h} are *linear*, this is called **linear programming**.
Otherwise **nonlinear programming**.

Optimization: Observations

Q: What if we are looking for a *maximizer* not a minimizer? *consider -f*
Give some examples:

- training ANNs
- robot path planning

What about multiple objectives?

- combine them
- look up Pareto optimal

Existence/Uniqueness

Terminology: **global minimum** / **local minimum**

Under what conditions on f can we say something about existence/uniqueness?

If $f : S \rightarrow \mathbb{R}$ is continuous on a closed and bounded set $S \subseteq \mathbb{R}^n$, then

a minimum exists.

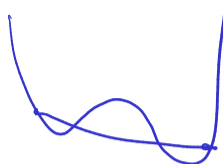
$f : S \rightarrow \mathbb{R}$ is called *coercive* on $S \subseteq \mathbb{R}^n$ (which must be unbounded) if

$$\lim_{\|x\| \rightarrow \infty} f(x) = +\infty$$

If f is coercive,

a global minimum.

Convexity



$S \subseteq \mathbb{R}^n$ is called **convex** if for all $x, y \in S$ and all $0 \leq \alpha \leq 1$

$$\alpha x + (1-\alpha)y \in S.$$

$f : S \rightarrow \mathbb{R}$ is called **convex on** $S \subseteq \mathbb{R}^n$ if for $x, y \in S$ and all $0 \leq \alpha \leq 1$

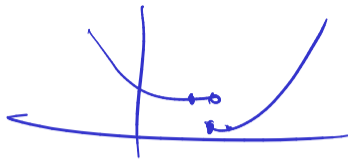
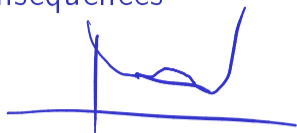
$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y)$$

Q: Give an example of a convex, but not **strictly convex** function.



→ likely non-uniqueness of the min.

Convexity: Consequences



If f is convex, ...

- f is continuous
- any local min is a global min.

If f is strictly convex, ...

any local min is a unique global min.

Optimality Conditions

$$f: \mathbb{R}^d \rightarrow \mathbb{R} \quad \nabla f = \nabla_x \in \mathbb{R}^{n \times 1}$$

If we have found a candidate x^* for a minimum, how do we know it actually is one? Assume f is smooth, i.e. has all needed derivatives.

1 in one-d:

Necessary: $f'(x^*) = 0$

Sufficient: $f'(x^*) = 0$ and $f''(x^*) > 0$
 \Rightarrow local min

In multiple-d:

necessary: $\nabla f = 0$

sufficient: $\nabla f = 0$ and $H_f(x^*)$ pos. def.

$$\frac{\partial^2 f}{\partial x_j \partial x_i}$$

Symm.



$$H_p = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} \end{pmatrix}$$

Optimization: Observations

Q: Come up with a hypothetical approach for finding minima.

Solve $\nabla f(x) = 0$ e.g. using Newton

Q: Is the Hessian symmetric?

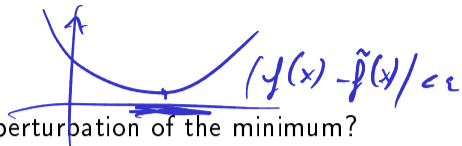
yes

Q: How can we practically test for positive definiteness?

Cholesky.

$$x^T A x > 0 \quad \wedge$$

Sensitivity and Conditioning (1D)



How does optimization react to a slight perturbation of the minimum?

$$f(x^* + h) = f(x^*) + \cancel{f'(x^*)h} + f'(x^*)\frac{h^2}{2} + O(h^3)$$

$$|x - x^*| \leq \sqrt{2\epsilon / f''(x^*)}$$

$$\text{If } \epsilon = 10^{-16} \Rightarrow \text{tol on solution is } 10^{-8}$$

Sensitivity and Conditioning (nD)

How does optimization react to a slight perturbation of the minimum?

