

Today

- non lin. h of
- optimization

Announcements

- HW8
- 4CH

Fixed Point Iteration

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

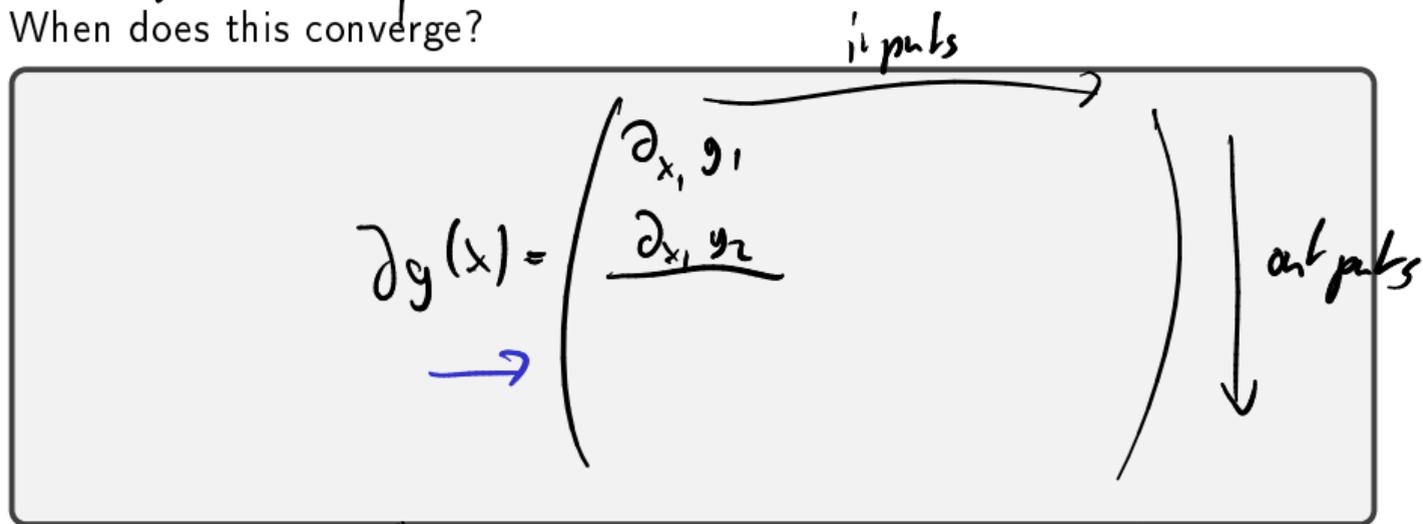
When does this converge?

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

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

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

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

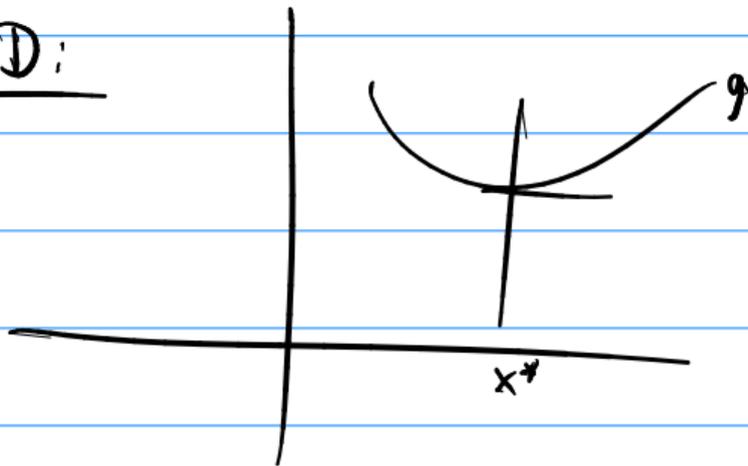


$$\|\partial g\|_p < 1 \Rightarrow \rho(\partial g(x^*)) < 1 \Rightarrow \text{lin. conv.}$$

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

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

1h 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?

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

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

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

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

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

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?

$$\frac{f(x + h\vec{e}_1) - f(x)}{h} \rightarrow \text{first column of } {}^n J_f^n$$

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

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.

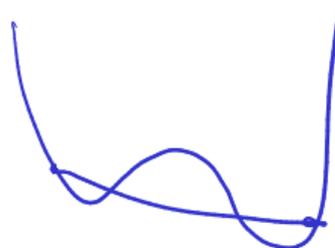
$f : S \rightarrow \mathbb{R}$ is called *coercive* on $S \subseteq \mathbb{R}^n$ (which must be unbounded) if

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

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 $0 \leq \alpha \leq 1$

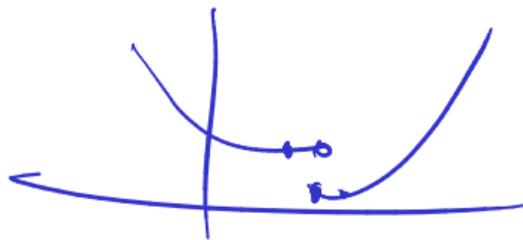
$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha)f(y)$$

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

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

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?

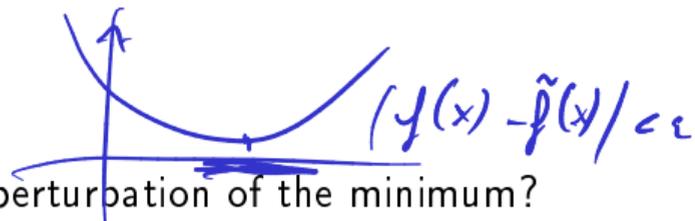
yes

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?

