Numerical Methods I: Nonlinear equations and nonlinear least squares

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Homework 2 due tomorrow morning, please hand in a printout, if possible.
Organization

- Homework 2 due tomorrow morning, please hand in a printout, if possible.
- Homework 3 to be posted tomorrow.
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Today: Review of linear least squares; Solving nonlinear equations; Nonlinear least squares problems
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Today: Review of linear least squares; Solving nonlinear equations; Nonlinear least squares problems

Questions?
Main reference:
Section 4 in Deuflhard/Hohmann.
Overview

Review of linear least squares and QR
Given data points/measurements

\[(t_i, b_i), \quad i = 1, \ldots, m\]

and a model function \(\phi\) that relates \(t\) and \(b\):

\[b = \phi(t; x_1, \ldots, x_n),\]

where \(x_1, \ldots, x_n\) are model function parameters. If the model is supposed to describe the data, the deviations/errors

\[\Delta_i = b_i - \phi(t_i, x_1, \ldots, x_n)\]

should be small. Thus, to fit the model to the measurements, one must choose \(x_1, \ldots, x_n\) appropriately.
We assume (for now) that the model depends linearly on \( x_1, \ldots, x_n \), e.g.:

\[
\phi(t; x_1, \ldots x_n) = a_1(t)x_1 + \ldots + a_n(t)x_n
\]

Choosing the least square error, this results in

\[
\min_x \|Ax - b\|,
\]

where \( x = (x_1, \ldots, x_n)^T \), \( b = (b_1, \ldots, b_m)^T \), and \( a_{ij} = a_j(t_i) \).

In the following, we study the over-determined case, i.e., \( m \geq n \).
Consider non-square matrices $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ and rank($A$) = $n$. Then the system

$$Ax = b$$

does, in general, not have a solution (more equations than unknowns). We thus instead solve a minimization problem

$$\min_{x} \|Ax - b\|^2.$$ 

The minimum $\bar{x}$ of this optimization problem is characterized by the normal equations:

$$A^T A \bar{x} = A^T b.$$
Solving the **normal equations**

\[ A^T A \bar{x} = A^T b \]

requires:

- computing \( A^T A \) (which is \( O(mn^2) \))
- condition number of \( A^T A \) is square of condition number of \( A \); (problematic for the Choleski factorization)
One would like to avoid the multiplication $A^TA$ and use a suitable factorization of $A$ that aids in solving the normal equation, the QR-factorization:

$$A = QR = [Q_1, Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1,$$

where $Q \in \mathbb{R}^{m \times m}$ is an orthonormal matrix ($QQ^T = I$), and $R \in \mathbb{R}^{m \times n}$ consists of an upper triangular matrix and a block of zeros.
How can the $QR$ factorization be used to solve the normal equation?

\[
\min_{x} \|Ax - b\|^2 = \min_{x} \|Q^T(Ax - b)\|^2 = \min_{x} \left\| \begin{bmatrix} b_1 - R_1x \\ b_2 \end{bmatrix} \right\|^2,
\]

where $Q^Tb = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$.

Thus, the least squares solution is $x = R^{-1}b_1$ and the residual is $\|b_2\|$.
Linear least-squares problems–QR factorization

How can we compute the QR factorization?

Givens rotations
Use sequence of rotations in 2D subspaces:
For $m \approx n$: $\sim n^2/2$ square roots, and $4/3n^3$ multiplications
For $m \gg n$: $\sim nm$ square roots, and $2mn^2$ multiplications

Householder reflections
Use sequence of reflections in 2D subspaces
For $m \approx n$: $2/3n^3$ multiplications
For $m \gg n$: $2mn^2$ multiplications

These methods compute an orthonormal basis of the columns of $A$. An alternative would be the Gram Schmidt method—however, Gram Schmidt is unstable and thus sensitive to rounding errors.
Nonlinear systems
Fixed point ideas

We intend to solve the nonlinear equation

\[ f(x) = 0, \quad x \in \mathbb{R}. \]

Reformulation as fixed point method:

\[ x = \Phi(x) \]

Corresponding iteration: Choose \( x_0 \) (initialization) and compute \( x_1, x_2, \ldots \) from

\[ x_{k+1} = \Phi(x_k) \]

When does this iteration converge?
Example: Solve the nonlinear equation

\[ 2x - \tan(x) = 0. \]

Iteration #1: \( x_{k+1} = \Phi_1(x_k) = 0.5 \tan(x_k) \)

Iteration #2: \( x_{k+1} = \Phi_2(x_k) = \arctan(2x_k) \)

Iteration #3: \( x_{k+1} = \Phi_3(x_k) = x_k - \frac{2x_k - \tan(x_k)}{1 - \tan^2(x_k)} \)
Convergence of fixed point methods

A mapping $\Phi : [a, b] \rightarrow \mathbb{R}$ is called contractive on $[a, b]$ if there is a $0 \leq \Theta < 1$ such that

$$|\Phi(x) - \Phi(y)| \leq \Theta|x - y| \text{ for all } x, y \in [a, b].$$

If $\Phi$ is continuously differentiable on $[a, b]$, then

$$\sup_{x, y \in [a, b]} \frac{|\Phi(x) - \Phi(y)|}{|x - y|} = \sup \limits_{z \in [a, b]} |\Phi'(z)|$$
Convergence of fixed point methods

Let $\Phi : [a, b] \rightarrow [a, b]$ be contractive with constant $\Theta < 1$. Then:

- There exists a unique fixed point $\bar{x}$ with $\bar{x} = \Phi(\bar{x})$
- For any starting guess $x_0$ in $[a, b]$, the fixed point iteration converges to $\bar{x}$ and

\[
|x_{k+1} - x_k| \leq \Theta|x_k - x_{k-1}| \quad \text{(linear convergence)}
\]

\[
|\bar{x} - x_k| \leq \frac{\Theta^k}{1 - \Theta}|x_1 - x_0|.
\]

The second expression allows to estimate the required number of iterations.
Newton’s method

In one dimension, solve $f(x) = 0$:

Start with $x_0$, and compute $x_1, x_2, \ldots$ from

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 0, 1, \ldots$$

Requires $f(x_k) \neq 0$ to be well-defined (i.e., tangent has nonzero slope).
Newton’s method

Let $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $n \geq 1$ and solve

$$F(x) = 0.$$ 

Taylor expansion about starting point $x^0$:

$$F(x) = F(x^0) + F'(x^0)(x - x^0) + o(|x - x^0|) \quad \text{for } x \rightarrow x^0.$$

Hence:

$$x^1 = x^0 - F'(x^0)^{-1}F(x^0)$$

**Newton iteration:** Start with $x^0 \in \mathbb{R}^n$, and for $k = 0, 1, \ldots$ compute

$$F'(x^k)\Delta x^k = -F(x^k), \quad x^{k+1} = x^k + \Delta x^k$$

Requires that $F'(x^k) \in \mathbb{R}^{n \times n}$ is invertible.

Newton’s method is **affine invariant**.
Convergence of Newton’s method

**Assumptions on \( F \):** \( D \subset \mathbb{R}^n \) open and convex, \( F : D \rightarrow \mathbb{R}^n \) continuously differentiable with \( F'(x) \) is invertible for all \( x \), and there exists \( \omega \geq 0 \) such that

\[
\| F'(x)^{-1}(F'(x + sv) - F'(x))v \| \leq s\omega \| v \|^2
\]

for all \( s \in [0, 1] \), \( x \in D \), \( v \in \mathbb{R}^n \) with \( x + v \in D \).

**Assumptions on \( x^* \) and \( x^0 \):** There exists a solution \( x^* \in D \) and a starting point \( x^0 \in D \) such that

\[
\rho := \| x^* - x^0 \| \leq \frac{2}{\omega} \quad \text{and} \quad B_\rho(x^*) \subset D
\]

**Theorem:** Then, the Newton sequence \( x^k \) stays in \( B_\rho(x^*) \) and

\[
\lim_{k \to \infty} x^k = x^*, \quad \text{and} \quad \| x^{k+1} - x^* \| \leq \frac{\omega}{2} \| x^k - x^* \|^2
\]
Newton’s method

Monotonicity test

\[ \| F(x^{k+1}) \| \leq \bar{\Theta} \| F(x^k) \|, \quad \bar{\Theta} < 1 \]
Newton’s method

Monotonicity test (affine invariant):

$$\|F'(x^k)^{-1}F(x^{k+1})\| \leq \bar{\Theta}\|F'(x^k)^{-1}F(x^k)\|, \quad \bar{\Theta} < 1$$
Newton’s method

Monotonicity test (affine invariant):

\[ \| F'(x^k)^{-1} F(x^{k+1}) \| \leq \tilde{\Theta} \| F'(x^k)^{-1} F(x^k) \|, \quad \tilde{\Theta} < 1 \]

Damping:

\[ x^{k+1} = x^k + \lambda_k \Delta x^k, \quad 0 < \lambda_k \leq 1 \]

For difficult problems, start with small \( \lambda_k \) and increase later in the iteration (close to the solution \( \lambda_k \) should be 1).
Newton’s method

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Approximative Jacobians: Use approximative Jacobians $\tilde{F}'(x^k)$, e.g., computed through finite differences.
Newton’s method

Convergence of Newton’s method

- The “more nonlinear” a problem, the harder it is to solve.
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Computation of Jacobian can be costly/complicated
Newton’s method
Convergence of Newton’s method

- The “more nonlinear” a problem, the harder it is to solve.
- **Computation of Jacobian** can be costly/complicated
- There’s **no reliable black-box solver** for nonlinear problems; at least for higher-dimensional problems, the structure of the problem must be taken into account.
Newton’s method
Convergence of Newton’s method

- The “more nonlinear” a problem, the harder it is to solve.
- Computation of Jacobian can be costly/complicated
- There’s no reliable black-box solver for nonlinear problems; at least for higher-dimensional problems, the structure of the problem must be taken into account.
- Sometimes, continuation ideas must be used to find good initializations: Solve simpler problems first and use solution as starting point for harder problems.
Choice of initialization $x^0$ is critical. Depending on the initialization, the Newton iteration might

- not converge (it could “blow up” or “oscillate” between two points)
- converge to different solutions
- fail cause it hits a point where the Jacobian is not invertible (this cannot happen if the conditions of the convergence theorem are satisfied)
- ...
Nonlinear versus linear problems

“Classification of mathematical problems as linear and nonlinear is like classification of the Universe as bananas and non-bananas.”
Nonlinear versus linear problems

“Classification of mathematical problems as linear and nonlinear is like classification of the Universe as bananas and non-bananas.”

or (according to Stanislav Ulam):

Using a term like nonlinear science is like referring to the bulk of zoology as the study of non-elephant animals.
Overview

Nonlinear least squares—Gauss-Newton
Nonlinear least-squares problems

Assume a least squares problem, where the parameters $\mathbf{x}$ do not enter linearly into the model. Instead of

$$\min_{\mathbf{x} \in \mathbb{R}^n} \| A\mathbf{x} - \mathbf{b} \|^2,$$

we have with $F : D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$:

$$\min_{\mathbf{x} \in \mathbb{R}^n} g(\mathbf{x}) := \frac{1}{2} \| F(\mathbf{x}) \|^2,$$

where $F(\mathbf{x})_i = \varphi(t_i, \mathbf{x}) - b_i$, $1 \leq i \leq m$

The (local) minimum $\mathbf{x}^*$ of this optimization problem satisfies:

$$g'(\mathbf{x}) = 0, \quad g''(\mathbf{x}) \text{ is positive definite.}$$
Nonlinear least-squares problems

The derivative of $g(\cdot)$ is

$$G(x) := g'(x) = F'(x)F(x)$$

This is a nonlinear system in $x$, $G : D \to \mathbb{R}^n$. Let’s try to solve it using Newton’s method:

$$G'(x^k)\Delta x^k = -G(x^k), \quad x^{k+1} = x^k + \Delta x^k$$

where

$$G''(x) = F'(x)^T F'(x) + F''^T(x)F(x).$$
Nonlinear least-squares problems

\( F''(x) \) is a tensor. It is often neglected due to the following reasons:

- It’s difficult to compute and we can use an approximate Jacobian in Newton’s method.
- If the data is compatible with the model, then \( F(x^*) = 0 \) and the term involving \( F''(x) \) drops out. If \( \|F(x^*)\| \) is small, neglecting that term might not make the convergence much slower.
- We know that \( g''(x^*) \) must be positive. If \( F'(x^k) \) has full rank, then \( F'(x)^T F'(x) \) is positive and invertible.
The resulting Newton method for the nonlinear least squares problem is called *Gauss-Newton method*: Initialize $x^0$ and for $k = 0, 1, \ldots$ solve

$$
F'(x^k)^T F'(x^k) \Delta x^k = -F'(x^k)^T F(x^k) \quad \text{(solve)}
$$

$$
x^{k+1} = x^k + \Delta x^k. \quad \text{(update step)}
$$
The resulting Newton method for the nonlinear least squares problem is called Gauss-Newton method: Initialize $x^0$ and for $k = 0, 1, \ldots$ solve

$$F'(x^k)^T F'(x^k) \Delta x^k = -F'(x^k)^T F(x^k) \quad \text{(solve)}$$

$$x^{k+1} = x^k + \Delta x^k. \quad \text{(update step)}$$

The solve step is the normal equation for the linear least squares problem

$$\min_{\Delta x} \| F'(x^k) \Delta x^k + F(x^k) \|.$$
Convergence of Gauss-Newton method

Assumptions on $F$: $D \subset \mathbb{R}^n$ open and convex, $F : D \to \mathbb{R}^m$, $m \geq n$ continuously differentiable with $F'(x)$ has full rank for all $x$, and let $\omega \geq 0$, $0 \leq \kappa^* < 1$ such that

$$\|F'(x) + (F'(x + sv) - F'(x))v\| \leq s\omega\|v\|^2$$

for all $s \in [0, 1]$, $x \in D$, $v \in \mathbb{R}^n$ with $x + v \in D$.

Assumptions on $x^*$ and $x^0$: Assume there exists a solution $x^* \in D$ of the least squares problem and a starting point $x^0 \in D$ such that

$$\|F'(x)^+ F(x^*)\| \leq \kappa^* \|x - x^*\|$$

$$\rho := \|x^* - x^0\| \leq \frac{2(1 - \kappa^*)}{\omega} := \sigma$$

Theorem: Then, the sequence $x^k$ stays in $B_\rho(x^*)$ and

$$\lim_{k \to \infty} x^k = x^*$$,

and

$$\|x^{k+1} - x^*\| \leq \frac{\omega}{2} \|x^k - x^*\|^2 + \kappa^* \|x^k - x^*\|$$
Convergence of Gauss-Newton method

- Role of $\kappa^*$: Represents omission of $F''(x)$
  - $\kappa^*$ can be chosen as 0 $\Rightarrow$ local quadratic convergence
  - $\kappa^* > 0$ linear convergence (thus we require $\kappa^* < 1$).

- Damping strategy as before (better: linesearch to make guaranteed progress in minimization problem)

- There can, in principle, be multiple solutions.
Nonlinear systems depending on parameters
Nonlinear systems depending on parameters

Consider

\[ F(x, \lambda) \quad \text{with} \quad F : \mathbb{R}^n \rightarrow \mathbb{R}^n, \]

where \( \lambda \) is one or a vector of parameters. This is a set of parametrized nonlinear systems. We would like to either

\[ \text{explore solution } x_{\lambda} \text{ for all } \lambda \text{ or find } x_{\lambda_0} \text{ for a specific } \lambda_0 \text{ that is difficult to solve directly} \]

Example:

\[ F(x, \lambda) = x (x^3 - x - \lambda). \]
Nonlinear systems depending on parameters

Consider

\[ F(x, \lambda) \text{ with } F : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n, \]

where \( \lambda \) is one or a vector of parameters. This is a set of parametrized nonlinear systems.
Nonlinear systems depending on parameters

Consider

\[ F(x, \lambda) \text{ with } F : \mathbb{R}^n \times \mathbb{R}^p \rightarrow \mathbb{R}^n, \]

where \( \lambda \) is one or a vector of parameters. This is a set of parametrized nonlinear systems.

We would like to either

- explore solution \( x_\lambda \) for all \( \lambda \) or
- find \( x_{\lambda_0} \) for a specific \( \lambda_0 \) that is difficult to solve directly using Newton’s method (e.g., solution to Navier Stokes with high Reynolds number)

Example:

\[ F(x, \lambda) = x(x^3 - x - \lambda). \]
Nonlinear systems depending on parameters

Regularity assumption:

\[ F'(x, \lambda) \text{ has full rank when } F(x, \lambda) = 0. \]

This excludes bifurcation points (due to the implicit function theorem). Study of bifurcation points (often very interesting!) requires additional work.

Continuation methods can exploit the local fast convergence of Newton’s method: Given solution \((x^0, \lambda_0, )\), find solution \((x^1, \lambda_1)\) for \(\lambda_1\) close to \(\lambda_0\).
Nonlinear systems depending on parameters

Continuation methods

- **Classical continuation:** Use $x^0$ as starting guess in Newton’s method for $\lambda_1$.

- **Tangent continuation:** Differentiate $F(x(s), \lambda_0 + s)$ with respect to $s$, and evaluate at $s = 0$. This leads to a better guess to initialize Newton’s method to find $x^1$.

These basic ideas additionally require some robustification to result in reliable algorithms; see Deuflhard/Hohmann.