Newton's Method and SuiteSparse

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Informatik 12:
Software and Tools for Computational Engineering

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Contents

Outline

Objective

- Introduction of an implementation of Newton's method for sparse problems based on the SuiteSparse matrix collection[1]

Learning Outcomes

- You will understand the construction of
  - a nonlinear residual with sparse Jacobian
  - a convex nonlinear objective with sparse Hessian.
- You will be able to
  - use and potentially extend the sample code.

[1] https://sparse.tamu.edu

Outline

We aim to construct

- a generic nonlinear residual $F : \boldsymbol{R}^n \rightarrow \boldsymbol{R}^n$ with invertible Jacobian $F' \in \boldsymbol{R}^{n \times n}$ whose sparsity pattern is defined by sample patterns in Matrix Market format from the SuiteSparse matrix collection.
- a generic nonlinear convex objective $f : \boldsymbol{R}^n \rightarrow \boldsymbol{R}$ with invertible Hessian $f'' \in \boldsymbol{R}^{n \times n}$ whose sparsity pattern is the same as that of F'.

to facilitate investigation of combinatorial problems due to sparse Jacobians and Hessians using a large number of different sparsity patterns.

It makes sense to start with the design of a generic nonlinear convex objective f followed by definition of the residual of the generic nonlinear system as the gradient of f, i.e, $F = f'$.

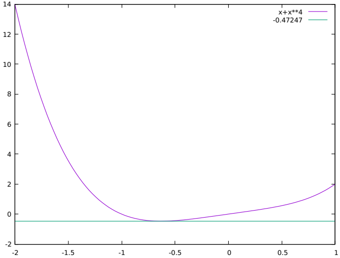
Outline

Toward Sparse Nonlinear Convex Objectives

Univariate Objective

We define $y = f(x) : \boldsymbol{R} \rightarrow \boldsymbol{R}$ as

$$y := x + x^4$$



yielding $y' = f'(x) \equiv \frac{df}{dx}(x) \in \boldsymbol{R}$ as

$$y' := 1 + 4 \cdot x^3$$

and $y'' = f''(x) \equiv \frac{d^2 f}{dx^2}(x) \in \boldsymbol{R}$ as

$$y'' := 12 \cdot x^2$$

and $y''' = f'''(x) \equiv \frac{d^3 f}{dx^3}(x) \in \boldsymbol{R}$ as

$$y''' := 24 \cdot x$$

We define $y = f(\mathbf{x}) : \boldsymbol{R}^n \rightarrow \boldsymbol{R}$ as

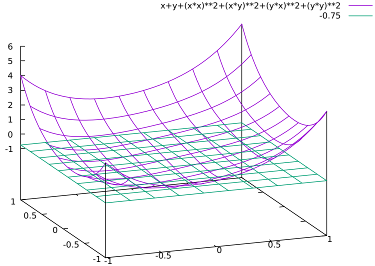
$$y := \mathbf{x}^T \cdot 1 + \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} (x_i \cdot x_j)^2$$

yielding $\mathbf{y}' = f'(\mathbf{x}) \equiv \frac{df}{d\mathbf{x}}(\mathbf{x}) \in \boldsymbol{R}^n$ as

$$\mathbf{y}' := 1 + 4 \cdot \mathbf{x}^T \cdot \mathbf{x} \cdot \mathbf{x} \, ,$$

and $Y'' = f''(\mathbf{x}) \equiv \frac{d^2 f}{d\mathbf{x}^2}(\mathbf{x}) \in \boldsymbol{R}^{n \times n}$ as

$$Y'' := 8 \cdot \mathbf{x} \cdot \mathbf{x}^T + 4 \cdot \mathbf{x}^T \cdot \mathbf{x} \cdot I_n \, .$$



Let $\mathcal{N} \subset \{0,\ldots,n-1\} \times \{0,\ldots,n-1\}\}$ denote index pairs of nonzero entries of the Hessian assuming nonzero diagonal entries. We define $y = f(\mathbf{x}) : \boldsymbol{R}^n \to \boldsymbol{R}$ as

$$\mathbf{y} := \mathbf{x}^T \cdot 1 + \sum_{(i,j)\in\mathcal{N}} (x_i \cdot x_j)^2$$

yielding $\mathbf{y}' = f'(\mathbf{x}) \equiv \frac{df}{d\mathbf{x}}(\mathbf{x}) \in \boldsymbol{R}^n$ as

$$\mathbf{y}' := 1; \quad \forall (i,j) \in \mathcal{N} : \begin{cases} y_i' := y_i' + 2 \cdot x_i \cdot x_j^2 \\ y_j' := y_j' + 2 \cdot x_i^2 \cdot x_j \end{cases}$$

and $Y'' = f''(\mathbf{x}) \equiv \frac{d^2 f}{d\mathbf{x}^2}(\mathbf{x}) \in \boldsymbol{R}^{n \times n}$ as

$$Y'' := 0; \quad \forall (i,j) \in \mathcal{N} : \begin{cases} Y''_{i,i} := Y''_{i,i} + 2 \cdot x_j^2 \\ Y''_{i,j} := Y''_{i,j} + 4 \cdot x_i \cdot x_j \\ Y''_{j,j} := Y''_{j,j} + 2 \cdot x_i^2 \\ Y''_{j,i} := Y''_{j,i} + 4 \cdot x_j \cdot x_i \end{cases}$$

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We define $y = f(x) : \boldsymbol{R} \rightarrow \boldsymbol{R}$ as

$$y := 1 + 4 \cdot x^3$$

yielding $y' = f'(x) \equiv \frac{df}{dx}(x) \in \boldsymbol{R}$ as

$$y' := 12 \cdot x^2$$

and $y'' = f''(x) \equiv \frac{d^2 f}{dx^2}(x) \in \boldsymbol{R}$ as

$$y'' := 24 \cdot x$$

See module Newton_I for implementation and background.

We define $\mathbf{y} = F(\mathbf{x}) : \boldsymbol{R}^n \rightarrow \boldsymbol{R}^n$ as

$$\mathbf{y} := 1 + 4 \cdot \mathbf{x}^T \cdot \mathbf{x} \cdot \mathbf{x} \,,$$

where $1 \equiv \sum_{i=0}^{n-1} \mathbf{e}_i$.

It follows $Y' = F'(\mathbf{x}) \equiv \frac{dF}{d\mathbf{x}}(\mathbf{x}) \in \boldsymbol{R}^{n \times n}$ as

$$Y' := 8 \cdot \mathbf{x} \cdot \mathbf{x}^T + 4 \cdot \mathbf{x}^T \cdot \mathbf{x} \cdot I_n \,.$$

See module Newton_II for implementation and background.

Let $\mathcal{N} \subset \{0,\ldots,n-1\} \times \{0,\ldots,n-1\}\}$ denote index pairs of nonzero entries of the Jacobian assuming nonzero diagonal entries.

We define $\mathbf{y} = F(\mathbf{x}) : \boldsymbol{R}^n \to \boldsymbol{R}^n$ as

$$\mathbf{y} := 1; \quad \forall (i,j) \in \mathcal{N} : \begin{cases} y_i := y_i + 2 \cdot x_i \cdot x_j^2 \\ y_j := y_j + 2 \cdot x_i^2 \cdot x_j \end{cases}$$

yielding $Y' = F'(\mathbf{x}) \equiv \frac{dF}{d\mathbf{x}}(\mathbf{x}) \in \boldsymbol{R}^{n \times n}$ as

$$Y' := 0; \quad \forall (i,j) \in \mathcal{N} : \begin{cases} Y'_{i,i} := Y'_{i,i} + 2 \cdot x_j^2 \\ Y'_{i,j} := Y'_{i,j} + 4 \cdot x_i \cdot x_j \\ Y'_{j,j} := Y'_{j,j} + 2 \cdot x_i^2 \\ Y'_{j,i} := Y'_{j,i} + 4 \cdot x_j \cdot x_i \end{cases}$$

Outline

Summary

- The sample code allows for use of sparsity patterns from the SuiteSparse matrix collection with Newton's method for nonlinear systems of equations as well as for nonlinear convex minimization problems.

Next Steps

- Get familiar with the sample code.
- Play with it, e.g, try different sparsity patterns from the SuiteSparse collection.
- Investigate convergence and run time.
- Continue the course to find out more ...