Newton-Krylov Methods for Expensive Nonlinear Function Evaluations

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The Problem

Find u^* such that $F(u^*) = 0$.

$u^* \in \Re^n$ **n is large**

***F* is nonlinear, and expensive to evaluate**

Introduction

Newton-Krylov methods are useful for solving large scale nonlinear problems. Key features include:

- Fast (quadratic) local convergence to a solution
- Do not require storage of the system Jacobian
  - more storage space available
  - able to solve bigger problems

Algorithm

u^k = current approx. to u^*

Form linear model for F:

$$\underbrace{F(\vec{u}^{k+1})}_{\text{want this } = 0} = F(\vec{u}^k) + \underbrace{J(\vec{u}^k)}_{\text{system Jacobian}} \underbrace{(\vec{u}^{k+1} - u^k)}_{=\vec{s}} \Rightarrow$$

$$J(\vec{u}^k)\vec{s} = -F(\vec{u}^k)$$

Approximate:

$$J(\vec{u}^k)\vec{s} \approx \frac{F(\vec{u}^k + \tau\vec{s}) - F(\vec{u}^k)}{\tau}$$

- Approximation does not change convergence rate
- $F(\vec{u}^k)$ can be saved, so only computed once
- $F(\vec{u}^k + \tau\vec{s})$ is calculated with each linear iteration
  - Very costly if F is expensive to evaluate!!

Solve the linear model for $\vec{s}$ using Krylov method (iterative)

Update:

$$\vec{u}^{k+1} = \vec{u}^k + \vec{s}$$

$$\vec{u}^k = \vec{u}^{k+1}$$

Is $F(\vec{u}^k) \approx 0$?

Yes → End

No → u^k = current approx. to u^*

Modifying for Expensive Nonlinear Functions

Replace $F(\vec{u}_k + \tau\vec{s})$ with $\tilde{F}(\vec{u}_k + \tau\vec{s})$ in the difference quotient only, where $F \approx \tilde{F}$, but $\tilde{F}$ is cheaper to evaluate.

- Theory shows careful choice of $\tilde{F}$ will not slow convergence
- Number of function evaluations dominated by calls made for difference quotient
  - Calls will be made to less expensive $\tilde{F}$
  - Expect less run time

Testing the Modified Method

We consider the system below which models predator-prey interaction for a number of species (ns):

$$F_i(\vec{u}) = \nabla \cdot D(u_i)\nabla u_i + f_i(x, y, \vec{u}) = 0, \; i = 1 \ldots ns$$

We solve for $\vec{u}$, which represents the species concentration over the domain, with u_i the concentration of the ith species, and $\hat{u}$ the approximation to u^* from the previous iteration.

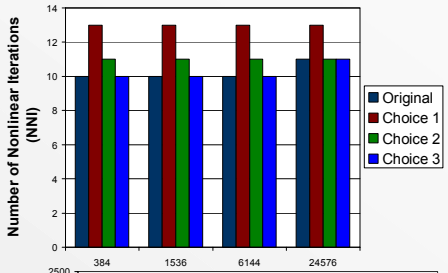
Three choices are made for $\tilde{F}$, by changing how $D(u_i) = d_i + 0.5u_i^2$ is computed:

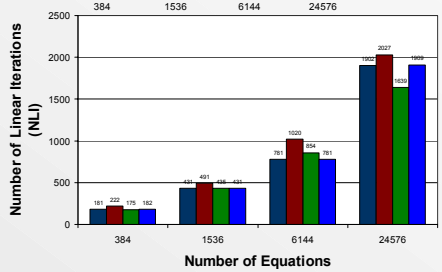
1. $\tilde{D} = D(\hat{u}_i)$ (cheapest, theory predicts poor performance)
2. $\tilde{D} = D(u_i, \hat{u}_i) = d_i + 0.5\hat{u}_i u_i$
3. $\tilde{D} = D(\hat{u}_i) + D'(\hat{u}_i)(u_i - \hat{u}_i)$ (most expensive, theory shows this choice will preserve convergence rate)

Preliminary Results

In the following figures, note:

- NNI (NLI) for **Choice 3** ≈ NNI (NLI) for **Original**
- Cheapest estimate, **Choice 1**, did poorly in comparison
- Interesting results for Choice 2 merit more investigation





Discussion

- Initial testing indicates modified difference quotient retains the local convergence properties, for at least some choices of approximating functions
- System function used for testing was not expensive to evaluate, so no direct evidence that this modification will decrease runtime
- Future tests on problems with more significant nonlinearities are planned to explore the issue of runtime savings

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