

Lecture 7: Gradient descent method

COMP5930M Scientific Computation

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Today

Recap

Algorithms for the initial state

Current strategies

Gradient descent (or steepest descent) method

The Newton algorithm

- ▶ Initial state: $\mathbf{x} = \mathbf{x}_0$
- ▶ while $|\mathbf{F}(\mathbf{x}_k)| > Tol$
 - ▶ $\mathbf{J}(\mathbf{x}_k)\delta = -\mathbf{F}(\mathbf{x}_k)$
 - ▶ $\mathbf{x}_{k+1} = \mathbf{x}_k + \lambda\delta$
- ▶ This first step is critical to the success of the algorithm

Guaranteeing convergence?

So far we have seen:

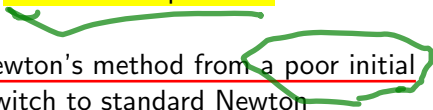
- ▶ Use domain-knowledge to choose \mathbf{x}_0
- ▶ Line-search update to improve convergence



Sometimes neither will lead to successful convergence

Gradient descent

- ▶ A solution algorithm in its own right
- ▶ Only linearly convergent
- ▶ Usually associated with minimisation problems
- ▶ Can be used to start Newton's method from a poor initial guess, after which we switch to standard Newton (similar idea as before when combining bisection and Newton)



Equivalence between minimisation and solving equations

- ▶ Given a system of nonlinear equations $\mathbf{F}(\mathbf{x}) = \mathbf{0}$, we can find an equivalent **optimisation problem**
- ▶ Define a new function $\phi(\mathbf{x}) = |\mathbf{F}|^2 = \sum_{i=1}^n (F_i(\mathbf{x}))^2$

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 - ▶ $\phi(\mathbf{x}) > 0, \forall \mathbf{x} \neq \mathbf{x}^*$
- ▶ Minimising ϕ is equivalent to finding a root of \mathbf{F}
- ▶ Optimality condition:

$$\nabla \phi(\mathbf{x}^*) = \frac{\partial}{\partial \mathbf{x}} \phi(\mathbf{x}^*) = \mathbf{0} \quad \Leftrightarrow \quad 2 J(\mathbf{x}^*)^T \mathbf{F}(\mathbf{x}^*) = \mathbf{0}.$$

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Proof of gradient formula

For each j :

$$\begin{aligned}\frac{\partial}{\partial x_j} \phi(\mathbf{x}) &= \frac{\partial}{\partial x_j} \sum_{i=1}^n (F_i(\mathbf{x}))^2 = 2 \sum_{i=1}^n \frac{\partial F_i}{\partial x_j}(\mathbf{x}) F_i(\mathbf{x}) \\ &= 2 \sum_{i=1}^n J_{ij}(\mathbf{x}) F_i(\mathbf{x}) = 2[J(\mathbf{x}^*)^T \mathbf{F}(\mathbf{x}^*)]_j\end{aligned}$$

The gradient

- ▶ Provided ϕ is differentiable we can define the gradient at our current solution point \mathbf{x}
$$\nabla\phi = \left(\frac{\partial\phi}{\partial x_1}, \frac{\partial\phi}{\partial x_2}, \dots, \frac{\partial\phi}{\partial x_n} \right)$$
- ▶ This defines a local vector direction, at \mathbf{x} , along which the function $\phi(\mathbf{x})$ increases most strongly
- ▶ Conversely, $\phi(\mathbf{x})$ decreases most strongly in the opposite direction $\mathbf{d} = -\nabla\phi$

Gradient descent algorithm

- ▶ Initial state: $\mathbf{x} = \mathbf{x}_0$
- ▶ while $|\mathbf{F}(\mathbf{x}_k)| > Tol$
 - ▶ Find descent direction: $\mathbf{d} = -2 \mathbf{J}^T(\mathbf{x}_k) \mathbf{F}(\mathbf{x}_k)$
 - ▶ Take descent step: $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}$
- ▶ We still require $\mathbf{J}(\mathbf{x}_k)$ at each iteration
- ▶ No linear system to solve, only matrix-vector multiplication
- ▶ No guarantee that $|\mathbf{F}(\mathbf{x}_{k+1})| < |\mathbf{F}(\mathbf{x}_k)|$, line-search required

Line search

- ▶ We have computed the direction to move \mathbf{d} but not the distance α
 - ▶ $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{d}$
- ▶ We can use a line search approach (see also last lecture)
 - ▶ In this case no upper limit on the distance $\alpha > 0$
 - ▶ Require descent steps $\phi(\mathbf{x}_{k+1}) < \phi(\mathbf{x}_k)$ as before
- ▶ More robust than Newton's Method, in particular for a poor initial guess
- ▶ Might converge only to a local minimum:

$$\nabla \phi(\mathbf{x}^*) = \mathbf{0}, \quad \text{but } \mathbf{F}(\mathbf{x}^*) \neq \mathbf{0}.$$

Gradient descent algorithm

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- ▶ while $|\mathbf{F}(\mathbf{x}_k)| > Tol$
 - ▶ $\mathbf{d} = -2 \mathbf{J}^T(\mathbf{x}_k) \mathbf{F}(\mathbf{x}_k)$
 - ▶ Perform line search to find optimal α
 - ▶ $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{d}$
- ▶ We still require $\mathbf{J}(\mathbf{x}_k)$ at each iteration
- ▶ No linear system to solve
- ▶ Must perform line search for α
- ▶ Newton $\delta = -J^{-1}\mathbf{F}$
Gradient descent $\mathbf{d} = -2J^T\mathbf{F}$



Notes on gradient descent

- ▶ Can be more aggressive
Increasing $\alpha > 1$ to move further
- ▶ Switching to Newton's Method?
(i) If gradient descent stalls, (ii) Once $\phi(\mathbf{x}_k) < tol_\phi$
Switch for faster convergence
- ▶ Typical failure case when $\phi(\mathbf{x})$ has flat regions and algorithm can't find a good step size \Rightarrow convergence stalls.