Lecture 18: Root-finding and minimization

STAT 545: Intro. to Computational Statistics

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Given some nonlinear function $f : \mathbb{R} \to \mathbb{R}$, solve

$$f(x) = 0$$

Invariably need iterative methods.

Assume f is continuous (else things are really messy).

More we know about f (e.g. gradients), better we can do.

Better: faster (asymptotic) convergence.

Root bracketing

$f(a)$ and $f(b)$ have opposite signs $\to$ root lies in (a, b).

a and b *bracket* the root.

Finding an initial bracketing can be non-trivial.
Typically, start with an initial interval and expand or contract.

Below, we assume we have an initial bracketing.

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Not always possible e.g. $f(x) = (x - a)^2$ (in general, multiple roots/nearby roots lead to trouble).

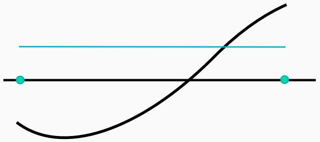
Bisection method

Simplest root-finding algorithm.

Given an initial bracketing, cannot fail.

But is slower than other methods.

Successively halves the bracketing interval (binary search):



- `Current interval =` (a, b)
- `Set` $c = \frac{a+b}{2}$
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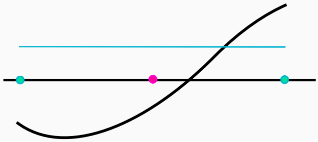

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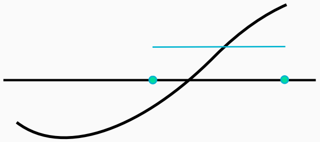

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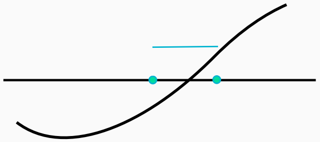

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Let ϵ_n be the interval length at iteration n.

Upperbounds error in root.

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- every (fixed) k iterations reduces error by one digit.
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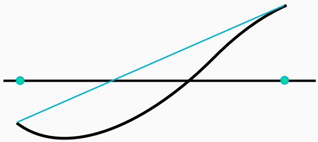
Superlinear convergence:

$$\lim_{n\to\infty} |\epsilon_{n+1}| = C \times |\epsilon_n|^m \qquad (m > 1)$$

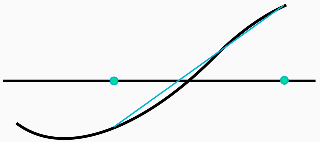
Quadratic convergence:
Number of significant figures *doubles* every iteration.

Linearly approximate f to find new approximation to root.



Secant method and bisection method

Linearly approximate f to find new approximation to root.

Secant method: 

- always keep the newest point
- Superlinear convergence ($m = 1.618$, the golden ratio)

$$\lim_{n\to\infty} |\epsilon_{n+1}| = C \times |\epsilon_n|^{1.618}$$

- Bracketing (and thus convergence) not guaranteed.

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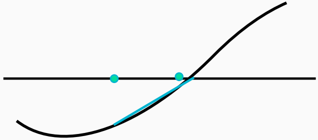

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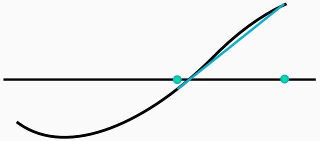

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False position:

- Can choose an old point that guarantees bracketing.
- Convergence analysis is harder.

Practical root-finding

In practice, people use more sophiticated algorithms.

Most popular is Brent's method.

Maintains bracketing by combining bisection method with a quadratic approximation.

Lots of book-keeping.

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At any point uses both function evaluation as well as derivative to form a linear approximation.

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$$0 = f(x_i) + \delta f'(x_i)$$

$$x_{i+1} = x_i - f(x_i)/f'(x_i)$$

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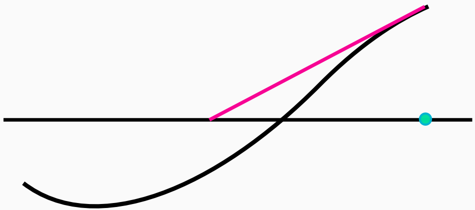

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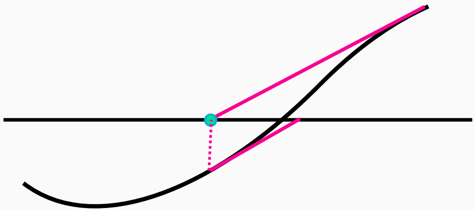

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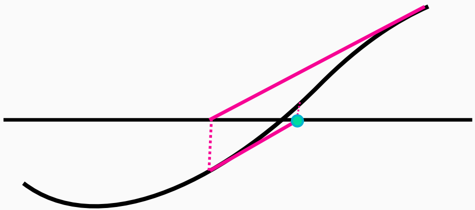

Convergence of Newton's method

Letting x be the root, we have

$$x_{i+1} - x = x_i - x - f(x_i)/f'(x_i)$$
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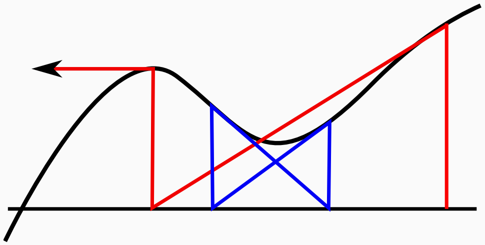
Quadratic convergence (assuming $f'(x)$ is non-zero at the root)

Pitfalls of Newton's method



Away from the root the linear approximation can be bad.

Can give crazy results (go off to infinity, cycles etc.)

However, once we have a decent solution can be used to rapidly 'polish the root'.

Often used in combination with some bracketing method.

Root-finding for systems of nonlinear equations

Find $(x_1, \cdots, x_N)$ such that:

$$F_i(x_1, \cdots, x_N) = 0 \qquad i = 1 \ to \ N$$

Much harder than the 1-d case.

Much harder than optimization.

Newton's method

Again, consider a Taylor expansion:

$$\mathbf{F}(\mathbf{x} + \delta\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J}(\mathbf{x}) \cdot \delta\mathbf{x} + O(\delta\mathbf{x}^2)$$

Here, $\mathbf{J}(\mathbf{x})$ is the Jacobian matrix at $\mathbf{x}$, with $J_{ij} = \frac{\partial F_i}{\partial x_j}$.

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$$\mathbf{J}(\mathbf{x}) \cdot \delta\mathbf{x} = -\mathbf{F}(\mathbf{x})$$

Solve e.g. by LU decomposition.

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Solve e.g. by LU decomposition.

Iterate $\mathbf{x}_{new} = \mathbf{x}_{old} + \delta\mathbf{x}$ until convergence.

Can wildly careen through space if not careful.

Global methods viq optimization

Recall, we want to solve $\mathsf{F}(\mathsf{x}) = 0 \quad (F_i(\mathsf{x}) = 0, \quad i = 1 \cdots N)$.

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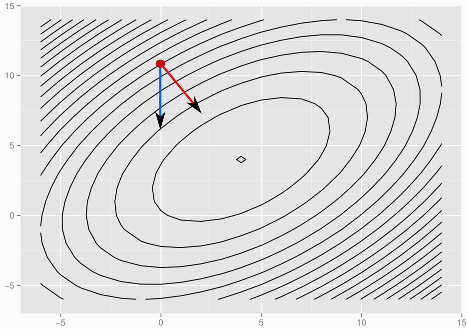
Minimize $f(\mathbf{x}) = \frac{1}{2}\sum_{i=1}^{N} |F_i(\mathbf{x})|^2 = \frac{1}{2}|\mathbf{F}(\mathbf{x})|^2 = \frac{1}{2}\mathbf{F}(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x})$.

Note: It is NOT sufficient to find a local minimum of f.

Global methods via optimization)

We move along $\delta \mathsf{x}$ instead of $\nabla f = \mathsf{F}(\mathsf{x})\mathsf{J}(\mathsf{x})$.

This keeps our global objective in sight.



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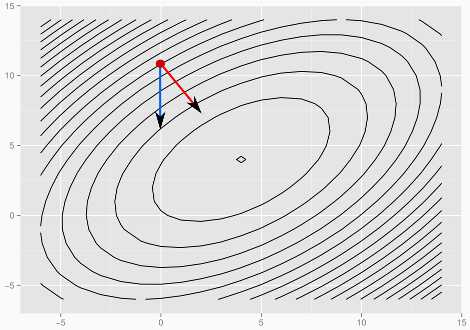

Note: $\nabla f \cdot \delta \mathsf{x} = (\mathsf{F}(\mathsf{x})\mathsf{J}(\mathsf{x})) \cdot (-\mathsf{J}^{-1}(\mathsf{x})\mathsf{F}(\mathsf{x})) = -\mathsf{F}(\mathsf{x})\mathsf{F}(\mathsf{x}) < 0$

Newton's method with backtracking

A full Newton step sets $\mathbf{x}_{new} = \mathbf{x}_{old} + \delta\mathbf{x}$.

This can cause f to increase i.e. $f(\mathbf{x}_{new} > f(\mathbf{x}_{old})$.

In this case, *backtrack* and set $\mathbf{x}_{new} = \mathbf{x}_{old} + \lambda\delta\mathbf{x}, \quad \lambda \in (0, 1)$.

Since $\delta\mathbf{x}$ is a descent direction, there exists a sufficiently small λ that causes f to decrease.

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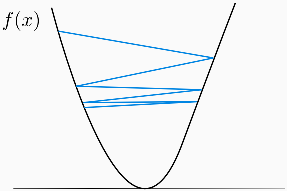
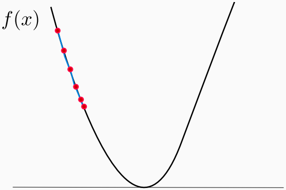
Finding best λ: too much work usually.

However, just causing f to decrease is not sufficient.

Wolfe conditions



Big steps with little decrease



Small steps getting us nowhere

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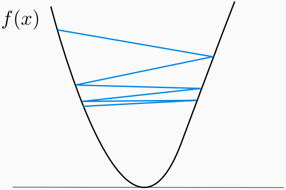

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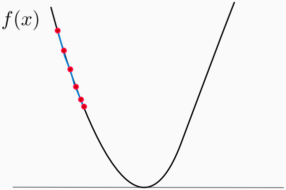
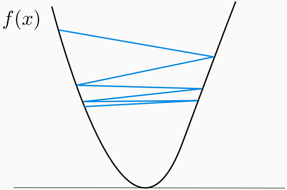


Small steps getting us nowhere

Avg. decrease at least some fraction of initial rate:

$$f(\mathbf{x} + \lambda\delta\mathbf{x}) \leq f(\mathbf{x}) + c_1\lambda(\nabla f \cdot \delta\mathbf{x}), \qquad c_1 \in (0, 1) \; e.g. \; 0.9$$



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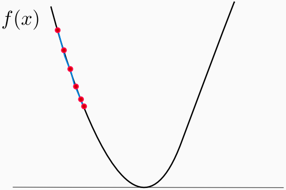

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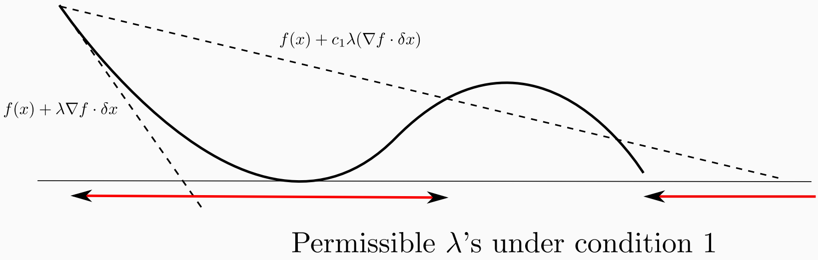
Final rate is greater than some fraction of initial rate:

$$\nabla f(\mathbf{x} + \lambda \delta \mathbf{x}) \cdot \delta \mathbf{x} \geq c_2 \nabla f(\mathbf{x}) \delta \mathbf{x}, \qquad c_2 \in (0,1) \; e.g. \; 0.1$$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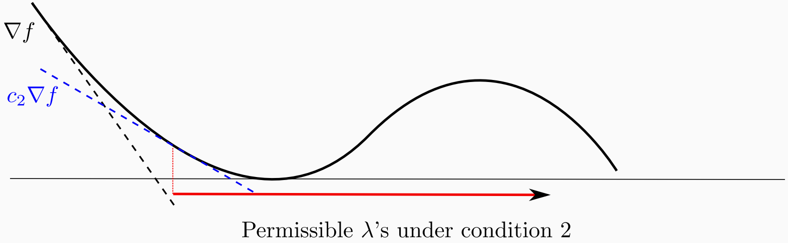
∇f
$c_2 \nabla f$
Permissible λ's under condition 2