Numerical Solutions of Nonlinear Systems of Equations (I)

- OPTIMIZATION is the foundation of MACHINE LEARNING.
  - SETUP: global search for optimal strategy:

$$\mathbf{min}_{\mathbf{x}\in\mathcal{R}^n} f\left(\mathbf{x}\right).$$

  - APPROACH: Optimal strategy satisfies non-linear equation

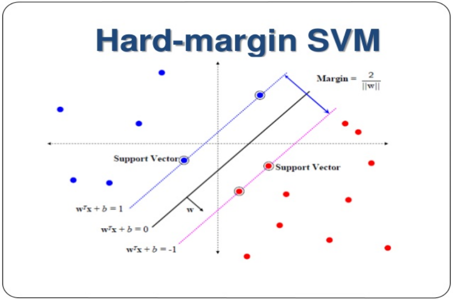
$$\nabla_{\mathbf{x}} f\left(\mathbf{x}\right) = \mathbf{0} \quad \in \mathcal{R}^n.$$

- Focus of Ch. 10, practical problems far harder

Numerical Solutions of Nonlinear Systems of Equations (II)

- **Ex:** Support Vector Machine (SVM) for classification:

$$\min_{\mathbf{w}\in\mathcal{R}^n,\ b\in\mathcal{R}} \left(\frac{1}{m} \left(\sum_{i=1}^{m} \max\left(0, 1 - y_i \left(\mathbf{w}^T \mathbf{x}_i - b\right)\right)\right) + \lambda \left\|\mathbf{w}\right\|_2^2 \right),$$



- Labels: $y_i = 1$ for blue, $y_i = -1$ for red.
- Solution requires more than nonlinear equations.

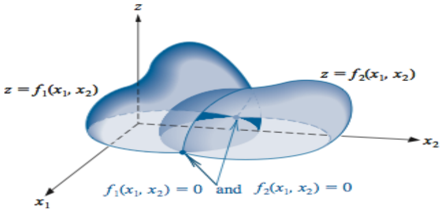
§10.1 Fixed Points for Functions of Several Variables

system of nonlinear equations has the form

$$\begin{aligned} f_1(x_1, x_2, \cdots, x_n) &= 0, \\ f_2(x_1, x_2, \cdots, x_n) &= 0, \\ &\vdots \\ f_n(x_1, x_2, \cdots, x_n) &= 0. \end{aligned}$$

In vector form

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}, \qquad \text{where } \mathbf{x} = (x_1, x_2, \cdots, x_n)^T.$$



Ex: Nonlinear equations

$$\begin{aligned} 3x_1 - \cos(x_2 x_3) &= \frac{1}{2}, \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 &= -1.06, \\ e^{-x_1 x_2} + 20x_3 &= -\frac{10\pi - 3}{3}. \end{aligned}$$

In vector form, with $\mathbf{x} = (x_1, x_2, x_3)^T$,

$$\mathbf{F}(\mathbf{x}) \stackrel{def}{=} \begin{pmatrix} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} \end{pmatrix} = \mathbf{0}.$$

Solution Methods

- Fixed Point Method
- Newton's Method
- Quasi-Newton Methods
- Steepest Descent Methods

Definitions

LIMIT: *Let f be defined on a set $\mathcal{D} \subset \mathcal{R}^n$ and mapping into $\mathcal{R}$.*

$\mathbf{lim}_{\mathbf{x} \to \mathbf{x}_0} f(\mathbf{x}) = L$ *if, given any number* $\epsilon > 0$,

a number $\delta > 0$ *exists with* $|f(\mathbf{x}) - L| < \epsilon$ *whenever* $\mathbf{x} \in \mathcal{D}$ *and* $0 < \|\mathbf{x} - \mathbf{x}_0| < \delta$.

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CONTINUOUS: *Function f is continuous at $\mathbf{x}_0 \in \mathcal{D}$ if*

$\mathbf{lim}_{\mathbf{x} \to \mathbf{x}_0} f(\mathbf{x})$ *exists and equals* $f(\mathbf{x}_0)$.

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CONTINUOUS: $\mathbf{F}(\mathbf{x}) \stackrel{def}{=} (f_1(\mathbf{x}), \cdots, f_n(\mathbf{x}))^T \in \mathcal{R}^n$ *is continuous on* $\mathcal{D}$, *or* $\mathbf{F} \in C(\mathcal{D})$, *if* $f_j(\mathbf{x}) \in C(\mathcal{D})$ *for* $j = 1, \cdots, n$.

Fixed Point in $\mathcal{R}^n$

Def: *Function* $\mathbf{G}(\mathbf{x}) : \mathcal{D} \subset \mathcal{R}^n \longrightarrow \mathcal{R}^n$ *has a* FIXED POINT *at* $\mathbf{p} \in \mathcal{D}$ *if* $\mathbf{G}(\mathbf{p}) = \mathbf{p}$.

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Thm: *Let* $\mathcal{D} = \left\{(x_1, \cdots, x_n)^T \mid \alpha_j \le x_j \le \beta_j,\ j = 1, \cdots, n.\right\}$. *Suppose* $\mathbf{G}(\mathbf{x}) \in C(\mathcal{D})$ *with the property that* $\mathbf{G}(\mathbf{x}) \in \mathcal{D}$ *whenever* $\mathbf{x} \in \mathcal{D}$. *Then* $\mathbf{G}$ *has a fixed point in* $\mathcal{D}$.

- **Ex:** nonlinear equations

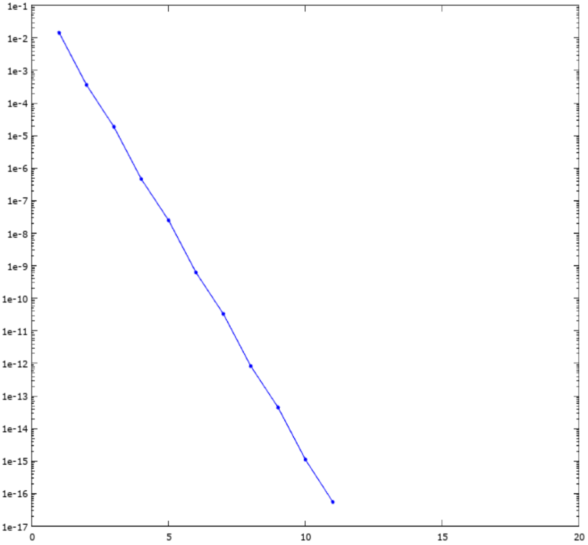
$$\mathbf{F}(\mathbf{x}) \overset{def}{=} \begin{pmatrix} 3x_1 - \cos(x_2x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2+0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1x_2} + 20x_3 + \frac{10\pi-3}{3} \end{pmatrix} = \mathbf{0}.$$

- **FPI 1:** $\mathbf{x} = \mathbf{G}_1(\mathbf{x})$:

$$\begin{aligned} x_1 &= \frac{1}{3}\cos(x_2x_3) + \frac{1}{6} \\ x_2 &= \frac{1}{9}\sqrt{x_1^2 + \sin x_3 + 1.06} - 0.1 \\ x_3 &= -\frac{1}{20}\left(e^{-x_1x_2} + \frac{10\pi-3}{3}\right) \end{aligned}$$

- $\mathbf{x}^{(0)} = (0,0,0)^T$ and FPT: $\mathbf{x}^{(k+1)} = \mathbf{G}_1\left(\mathbf{x}^{(k)}\right),\ k = 0, 1, \cdots$

Fixed Point Iteration, $x_0 = (0,0,0)^T$, $FT = (0.5, 0, -\pi/6)^T$



- **Ex:** nonlinear equations

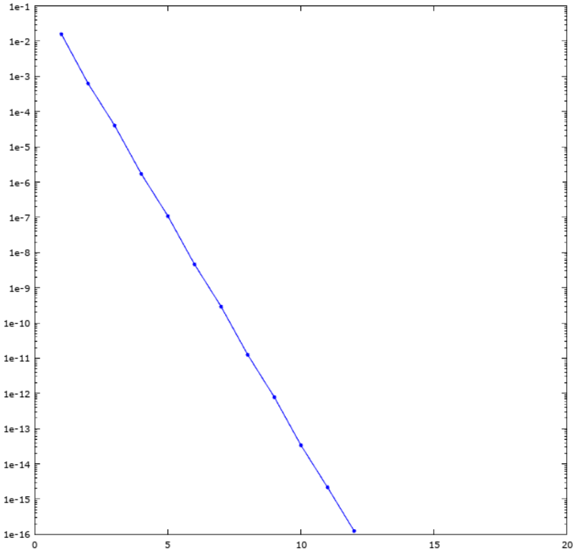
$$\mathbf{F}(\mathbf{x}) \stackrel{def}{=} \begin{pmatrix} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} \end{pmatrix} = \mathbf{0}.$$

- **FPI 2:** $\mathbf{x} = \mathbf{G}_2(\mathbf{x})$:

$$\begin{aligned} x_1 &= \frac{1}{3}\cos(x_2 x_3) + \frac{1}{6} \\ x_2 &= -\frac{1}{9}\sqrt{x_1^2 + \sin x_3 + 1.06} - 0.1 \\ x_3 &= -\frac{1}{20}\left(e^{-x_1 x_2} + \frac{10\pi - 3}{3}\right) \end{aligned}$$

- $\mathbf{x}^{(0)} = (0, 0, 0)^T$ and FPT: $\mathbf{x}^{(k+1)} = \mathbf{G}_2\left(\mathbf{x}^{(k)}\right)$, $k = 0, 1, \cdots$

$x_0 = (0,0,0)^T$, FT = $(0.49814 \ \ -0.19961 \ \ -0.52883)^T$



Let $\mathcal{D} = \left\{ (x_1, \cdots, x_n)^T \mid \alpha_j \le x_j \le \beta_j,\ j = 1, \cdots, n. \right\}$. Suppose $\mathbf{G}(\mathbf{x}) \in C(\mathcal{D})$ with the property that $\mathbf{G}(\mathbf{x}) \in \mathcal{D}$ whenever $\mathbf{x} \in \mathcal{D}$.

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Thm: Let $\mathcal{J}(\mathbf{x}) \stackrel{def}{=} \left(\frac{\partial g_i(\mathbf{x})}{\partial x_j} \right)$. Assume that there exists a constant $\kappa < 1$ so that $\|\mathcal{J}(\mathbf{x})\|_\infty \le \kappa$ for all $\mathbf{x} \in \mathcal{D}$. Then FPI

$$\mathbf{x}^{(k+1)} = \mathbf{G}\left(\mathbf{x}^{(k)}\right), \quad k = 0, 1, \cdots$$

with $\mathbf{x}^{(0)} \in \mathcal{D}$ converges to the unique FP $\mathbf{p} \in \mathcal{D}$ and

$$\left\| \mathbf{x}^{(k)} - \mathbf{p} \right\|_\infty \le \frac{\kappa^k}{1-\kappa} \left\| \mathbf{x}^{(0)} - \mathbf{p} \right\|_\infty .$$

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$$\left\|\mathbf{x}^{(k)} - \mathbf{p}\right\|_\infty \le \frac{\kappa^k}{1-\kappa} \left\|\mathbf{x}^{(0)} - \mathbf{p}\right\|_\infty .$$

Thm: If $\mathcal{J}(\mathbf{p}) = 0$ and $\left| \frac{\partial^2 g_i(\mathbf{x})}{\partial x_j \partial x_t} \right| \le M$ for all $1 \le i, j, t \le n$. Then for sufficiently large k,

$$\left\|\mathbf{x}^{(k)} - \mathbf{p}\right\|_\infty \le \frac{n^2 M}{2} \left\|\mathbf{x}^{(k-1)} - \mathbf{p}\right\|_\infty^2 .$$

§10.2 Newton's Method: one-dimensional case review

To solve $f(x) = 0$, consider fixed point function for some function $\phi(x)$:

$$g(x) = x - \phi(x)\, f(x).$$

- Let p be a root for $f(x)$: $f(p) = 0$.
- Then p is fixed point for $g(x)$: $p = g(p)$.
- At fixed point p: $g'(p) = 1 - \phi(p)\, f'(p)$.
- For quadratic convergence, need to choose $\phi(x)$ so $g'(p) = 0$, or $\phi(p) = \frac{1}{f'(p)}$.
- Newton's method

$$x^{(k+1)} = g\left(x^{(k)}\right), \quad k = 0, 1, \cdots$$

with $g(x) = x - \frac{f(x)}{f'(x)}$.

§10.2 Newton's Method: *n*-dimensional case

To solve $\mathbf{F}(\mathbf{x}) = \mathbf{0} \in \mathcal{R}^n$, consider fixed point function for some matrix function $\mathcal{A}(\mathbf{x}) \in \mathcal{R}^{n \times n}$:

$$\mathbf{G}(\mathbf{x}) = \mathbf{x} - \mathcal{A}(\mathbf{x})^{-1} \, \mathbf{F}(\mathbf{x}).$$

- Let $\mathbf{p}$ be a root for $\mathbf{F}(\mathbf{x})$: $\mathbf{F}(\mathbf{p}) = \mathbf{0}$.
- Then $\mathbf{p}$ is fixed point for $\mathbf{G}(\mathbf{x})$: $\mathbf{p} = \mathbf{G}(\mathbf{p})$.
- At fixed point $\mathbf{p}$: $\mathcal{J}_{\mathbf{x}}(\mathbf{G}(\mathbf{p})) = I - \mathcal{A}(\mathbf{p})^{-1} \, \mathcal{J}_{\mathbf{x}}(\mathbf{F}(\mathbf{p}))$.
- For quadratic convergence, need to choose $\mathcal{A}(\mathbf{x})$ so $\mathcal{J}_{\mathbf{x}}(\mathbf{G}(\mathbf{p})) = \mathbf{0}$, or $\mathcal{A}(\mathbf{p}) = \mathcal{J}_{\mathbf{x}}(\mathbf{F}(\mathbf{p}))$.
- Newton's method

$$x^{(k+1)} = \mathbf{G}\left(\mathbf{x}^{(k)}\right), \quad k = 0, 1, \cdots$$

with $\mathbf{G}(\mathbf{x}) = \mathbf{x} - \mathcal{J}_{\mathbf{x}}^{-1}(\mathbf{F}(\mathbf{x})) \, \mathbf{F}(\mathbf{x})$.

Ex: Nonlinear equations with $\mathbf{x} = (x_1, x_2, x_3)^T$,

$$\mathbf{F}(\mathbf{x}) \stackrel{def}{=} \begin{pmatrix} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} \end{pmatrix} = \mathbf{0}.$$

Jacobian matrix has analytic form:

$$\mathcal{J}_{\mathbf{x}}(\mathbf{F}(\mathbf{x})) = \begin{pmatrix} 3 & x_3 \sin(x_2 x_3) & x_2 \sin(x_2 x_3) \\ 2\,x_1 & -162(x_2 + 0.1) & \cos x_3 \\ -x_2\, e^{-x_1 x_2} & -x_1\, e^{-x_1 x_2} & 20 \end{pmatrix}.$$

Newton's method with $\mathbf{x}^{(0)} = (0.1, 0.1, -0.1)^T$

k	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$\|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|_\infty$
0	0.1000000000	0.1000000000	−0.1000000000	
1	0.4998696728	0.0194668485	−0.5215204718	0.4215204718
2	0.5000142403	0.0015885914	−0.5235569638	1.788×10^{-2}
3	0.5000000113	0.0000124448	−0.5235984500	1.576×10^{-3}
4	0.5000000000	8.516×10^{-10}	−0.5235987755	1.244×10^{-5}
5	0.5000000000	-1.375×10^{-11}	−0.5235987756	8.654×10^{-10}

§10.2 Quasi-Newton Method: Broyden Method

MOTIVATION: Newton's method costs too much for large n.
Quasi-Newton Method: poor man's alternative.

- Newton's method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathcal{A}\left(\mathbf{x}^{(k)}\right)^{-1} \mathbf{F}\left(\mathbf{x}^{(k)}\right), \quad \text{where} \quad \mathcal{A}(\mathbf{x}) = \left(\frac{\partial f_i(\mathbf{x})}{\partial x_j}\right)$$

- PROBLEM I WITH NEWTON: Requires n^2 partial derivatives.
- PROBLEM II WITH NEWTON: Needs to factorize $\mathcal{A}\left(\mathbf{x}^{(k)}\right)$ for each k.

Something cheaper, for slower convergence but less overall computation

Broyden Method: Motivation

- Broyden Method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathcal{A}_k^{-1}\,\mathbf{F}\left(\mathbf{x}^{(k)}\right), \quad \text{where} \quad \mathcal{A}_k \in \mathcal{R}^{n\times n}.$$

- DESIRED PROPERTY I: "Mimics" $\mathcal{A}\left(\mathbf{x}^{(k)}\right)$ in some sense.
- DESIRED PROPERTY II: "Easy" to compute $\mathcal{A}_{k+1}^{-1}$ from $\mathcal{A}_k^{-1}$.

Broyden Method: Derivation

- Assume for some step $k \geq 0$, we have available $\mathbf{x}^{(k)} \in \mathcal{R}^n$ and $\mathcal{A}_k \in \mathcal{R}^{n \times n}$. By Broyden Method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathcal{A}_k^{-1} \mathbf{F}\left(\mathbf{x}^{(k)}\right).$$

- Secant equation

$$\mathbf{F}\left(\mathbf{x}^{(k+1)}\right) - \mathbf{F}\left(\mathbf{x}^{(k)}\right) \approx \mathcal{A}\left(\mathbf{x}^{(k)}\right)\left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right).$$

- Broyden ideas:
  - Approximate secant equation: $\mathcal{A}_{k+1}\, \mathbf{s}_{k+1} = \mathbf{y}_{k+1}$, where

$$\mathbf{y}_{k+1} \stackrel{def}{=} \mathbf{F}\left(\mathbf{x}^{(k+1)}\right) - \mathbf{F}\left(\mathbf{x}^{(k)}\right), \quad \mathbf{s}_{k+1} \stackrel{def}{=} \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}.$$

  - Choose a special $\mathcal{A}_{k+1}$ that does not differ much from $\mathcal{A}_k$

$$\mathcal{A}_{k+1} = \mathcal{A}_k + \frac{\mathbf{y}_{k+1} - \mathcal{A}_k\, \mathbf{s}_{k+1}}{\left\|\mathbf{s}_{k+1}\right\|_2^2} \mathbf{s}_{k+1}^T$$

Broyden Method

- Initialization: Given $\mathbf{x}^{(0)} \in \mathcal{R}^n$.
- Choose $\mathcal{A}_0 \in \mathcal{R}^{n \times n}$.
- For $k = 0, 1, \cdots,$

$$
\begin{aligned}
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} - \mathcal{A}_k^{-1} \mathbf{F}\left(\mathbf{x}^{(k)}\right), \\
\mathcal{A}_{k+1} &= \mathcal{A}_k + \frac{\mathbf{y}_{k+1} - \mathcal{A}_k \, \mathbf{s}_{k+1}}{\|\mathbf{s}_{k+1}\|_2^2} \mathbf{s}_{k+1}^T, \quad \text{with}
\end{aligned}
$$

$$
\mathbf{y}_{k+1} = \mathbf{F}\left(\mathbf{x}^{(k+1)}\right) - \mathbf{F}\left(\mathbf{x}^{(k)}\right), \quad \mathbf{s}_{k+1} = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}.
$$

Broyden Method

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- Choose $\mathcal{A}_0 \in \mathcal{R}^{n \times n}$.
- For $k = 0, 1, \cdots$,

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$$\mathbf{y}_{k+1} = \mathbf{F}\left(\mathbf{x}^{(k+1)}\right) - \mathbf{F}\left(\mathbf{x}^{(k)}\right), \quad \mathbf{s}_{k+1} = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}.$$

Practical details:

- $\mathcal{A}_k^{-1}$ may not exist. (Broyden method fails)
- Does an LU factorization of $\mathcal{A}_k$ help when we compute LU factorization of $\mathcal{A}_{k+1}$? (Yes, but another story)
- If $\mathcal{A}_k^{-1}$ does exist and is available,

$$\mathcal{A}_{k+1}^{-1} = \mathcal{A}_k^{-1} + \frac{\mathbf{s}_{k+1} - \mathcal{A}_k^{-1} \mathbf{y}_{k+1}}{\mathbf{s}_{k+1}^T \mathcal{A}_k^{-1} \mathbf{y}_{k+1}} \mathbf{s}_{k+1}^T \mathcal{A}_k^{-1}.$$

Ex: Nonlinear equations with $\mathbf{x} = (x_1, x_2, x_3)^T$,

$$\mathbf{F}(\mathbf{x}) \stackrel{def}{=} \begin{pmatrix} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} \end{pmatrix} = \mathbf{0}.$$

Jacobian matrix has analytic form:

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Quasi-Newton method with $\mathbf{x}^{(0)} = (0.1, 0.1, -0.1)^T$,
$\mathcal{A}_0 = \mathcal{J}_{\mathbf{x}}\left(\mathbf{F}\left(\mathbf{x}^{(0)}\right)\right)$

k	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$\Vert\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\Vert_2$
3	0.5000066	8.672157×10^{-4}	−0.5236918	7.88×10^{-3}
4	0.5000003	6.083352×10^{-5}	−0.5235954	8.12×10^{-4}
5	0.5000000	-1.448889×10^{-6}	−0.5235989	6.24×10^{-5}
6	0.5000000	6.059030×10^{-9}	−0.5235988	1.50×10^{-6}

§10.4 Steepest Descent Techniques (I)

System of nonlinear equations has the form

$$\begin{aligned} f_1(x_1, x_2, \cdots, x_n) &= 0, \\ f_2(x_1, x_2, \cdots, x_n) &= 0, \\ &\vdots \\ f_n(x_1, x_2, \cdots, x_n) &= 0. \end{aligned}$$

In vector form, with $\mathbf{x} = (x_1, x_2, \cdots, x_n)^T$:

$$\mathbf{F}(\mathbf{x}) \overset{def}{=} \begin{pmatrix} f_1(x_1, x_2, \cdots, x_n) \\ f_2(x_1, x_2, \cdots, x_n) \\ \vdots \\ f_n(x_1, x_2, \cdots, x_n) \end{pmatrix} = \mathbf{0}, \quad .$$

Def: $g(\mathbf{x}) \overset{def}{=} \mathbf{F}(\mathbf{x})^T \ \mathbf{F}(\mathbf{x}) = \sum_{j=1}^{n} f_j^2(x_1, x_2, \cdots, x_n)$. Then

$$\mathbf{F}(\mathbf{x}) = \mathbf{0} \iff \mathbf{min}_{\mathbf{x} \in \mathcal{R}^n} g(\mathbf{x}) = 0.$$

Steepest Descent Techniques (II)

$g(\mathbf{x}) \stackrel{def}{=} \mathbf{F}(\mathbf{x})^T \; \mathbf{F}(\mathbf{x}) = \sum_{j=1}^{n} f_j^2(x_1, x_2, \cdots, x_n)$. Then

$$\mathbf{F}(\mathbf{x}) = \mathbf{0} \iff \mathbf{min}_{\mathbf{x}\in\mathcal{R}^n} g(\mathbf{x}) = 0.$$

Algorithm 1 Generic Descent Algorithm

Evaluate $g(\mathbf{x})$ at an initial approximation vector $\mathbf{x}^{(0)} \in \mathcal{R}^n$.
Set $k = 0$.
while NOT YET CONVERGED **do**
  Determine a direction $\mathbf{d}^{(k)}$ from $\mathbf{x}^{(k)}$ that results in a decrease in the value of $g(\mathbf{x})$ (DESCENT DIRECTION.)
  Move an appropriate amount α (STEP-SIZE) in this direction:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha\, \mathbf{d}^{(k)}.$$

  $k = k + 1$
end while

Gradient and descent directions

Gradient: $\nabla_{\mathbf{x}} g(\mathbf{x}) = \begin{pmatrix} \frac{\partial g(\mathbf{x})}{\partial x_1} \\ \vdots \\ \frac{\partial g(\mathbf{x})}{\partial x_n} \end{pmatrix}.$

Directional deriv:

$$\mathcal{D}_{\mathbf{v}} g(\mathbf{x}) \stackrel{def}{=} \lim_{h \longrightarrow 0} \frac{g(\mathbf{x} + h\,\mathbf{v}) - g(\mathbf{x})}{h} = \mathbf{v}^T \nabla_{\mathbf{x}} g(\mathbf{x}).$$

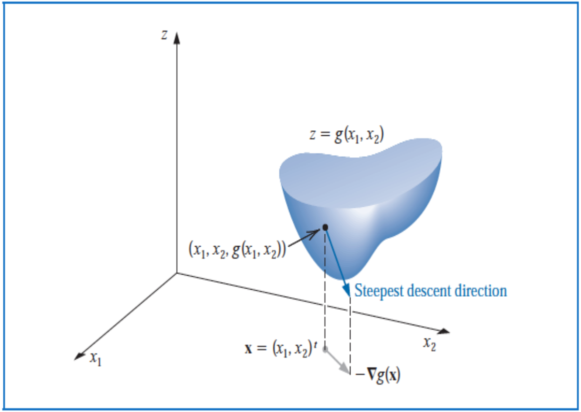
Steepest descent: *For any* $\|\mathbf{v}\|_2 = 1$ *and tiny* $\alpha > 0$*:*

$$\begin{aligned} g(\mathbf{x} - \alpha\,\mathbf{v}) &= g(\mathbf{x}) - \alpha\,\mathbf{v}^T \nabla_{\mathbf{x}} g(\mathbf{x}) + O\left(\alpha^2\right) \\ &\geq g(\mathbf{x}) - \alpha\,\|\nabla_{\mathbf{x}} g(\mathbf{x})\|_2 + O\left(\alpha^2\right). \end{aligned}$$

$g(\mathbf{x} - \alpha\,\mathbf{v})$ decreases asymptotically the most with $\mathbf{v} = \frac{\nabla_{\mathbf{x}} g(\mathbf{x})}{\|\nabla_{\mathbf{x}} g(\mathbf{x})\|_2}$

Steepest descent

$$g\left(\mathbf{x} - \alpha\,\nabla_{\mathbf{x}} g\left(\mathbf{x}\right)\right) \approx g\left(\mathbf{x}\right) - \alpha\,\left\|\nabla_{\mathbf{x}} g\left(\mathbf{x}\right)\right\|_2^2 .$$



Steepest Descent Algorithm for solving $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ (I)

Algorithm 2 Steepest Descent Algorithm

Evaluate $g(\mathbf{x}) \overset{def}{=} \|\mathbf{F}(\mathbf{x})\|_2^2$ at initial vector $\mathbf{x}^{(0)} \in \mathcal{R}^n$. Set $k = 0$.
while NOT YET CONVERGED **do**
  Set $\mathbf{d}^{(k)} = -\nabla_{\mathbf{x}} g(\mathbf{x}) = -2\left(\mathcal{J}(\mathbf{F}(\mathbf{x}))\right)^T \mathbf{F}(\mathbf{x})$.
  Move an appropriate amount α (STEP-SIZE) in this direction:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha\, \mathbf{d}^{(k)}.$$

  $k = k + 1$
end while

Algorithm 2 allows many different choices for α_k

- α should be "cheap" to compute.
- α should ensure "sufficient" reduction in $g(\mathbf{x})$.

Step-size Selection

- Ensure reduction in $g(\mathbf{x})$: Algorithm 3 will halt with an $\alpha_3 > 0$ so that $g\left(\mathbf{x}^{(k)} + \alpha_3 \mathbf{d}^{(k)}\right) < g\left(\mathbf{x}^{(k)}\right)$.

Algorithm 3 $g(\mathbf{x})$ Reduction

Set $\alpha_3 = 1$.
while $g\left(\mathbf{x}^{(k)} + \alpha_3 \mathbf{d}^{(k)}\right) \geq g\left(\mathbf{x}^{(k)}\right)$ **do**
  Set $\alpha_3 = \frac{\alpha_3}{2}$.
end while

Step-size Selection

- Ensure reduction in $g(\mathbf{x})$: Algorithm 3 will halt with an $\alpha_3 > 0$ so that $g\left(\mathbf{x}^{(k)} + \alpha_3\,\mathbf{d}^{(k)}\right) < g\left(\mathbf{x}^{(k)}\right)$.

Algorithm 3 $g(\mathbf{x})$ Reduction

Set $\alpha_3 = 1$.
while $g\left(\mathbf{x}^{(k)} + \alpha_3\,\mathbf{d}^{(k)}\right) \geq g\left(\mathbf{x}^{(k)}\right)$ **do**
  Set $\alpha_3 = \frac{\alpha_3}{2}$.
end while

- Ensure SUFFICIENT reduction in $g(\mathbf{x})$ with $\alpha^{(k)}$:

Algorithm 4 $g(\mathbf{x})$ Sufficient Reduction

Set $\alpha_2 = \alpha_3/2$. Compute coefficients h_0, h_1, h_2 so $\mathbf{P}(\alpha) = h_0 + h_1\,\alpha + h_2\,\alpha\,(\alpha - \alpha_2)$ interpolates $g\left(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)}\right)$ at $\alpha = 0, \alpha_2, \alpha_3$. Set $\alpha_0 = \frac{1}{2}(\alpha_2 - h_1/h_2)$

$$\alpha^{(k)} = \mathbf{argmin}_{\alpha \in [\alpha_0, \alpha_2, \alpha_3]} g\left(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)}\right).$$

Steepest Descent Algorithm for solving $\mathbf{F}(\mathbf{x}) = \mathbf{0}$ (II)

Algorithm 5 Steepest Descent Algorithm

Evaluate $g(\mathbf{x}) \stackrel{def}{=} \|\mathbf{F}(\mathbf{x})\|_2^2$ at initial vector $\mathbf{x}^{(0)} \in \mathcal{R}^n$. Set $k = 0$.
while NOT YET CONVERGED **do**
  Set $\mathbf{d}^{(k)} = -\nabla_{\mathbf{x}} g(\mathbf{x}) = -2\left(\mathcal{J}(\mathbf{F}(\mathbf{x}))\right)^T \mathbf{F}(\mathbf{x})$,
  $\mathbf{d}^{(k)} = \mathbf{d}^{(k)} / \left\|\mathbf{d}^{(k)}\right\|_2$,   (<u>bad move</u>)
  Compute $\alpha^{(k)}$ with Algorithms 3 and 4.

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)}.$$

  $k = k + 1$
end while

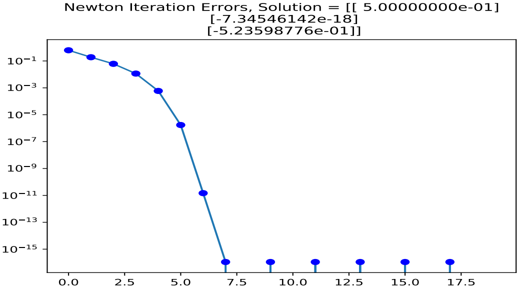
Ex: Nonlinear equations with $\mathbf{x} = (x_1, x_2, x_3)^T$,

$$\mathbf{F}(\mathbf{x}) \stackrel{def}{=} \left(\begin{array}{l} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} \end{array} \right) = \mathbf{0}.$$

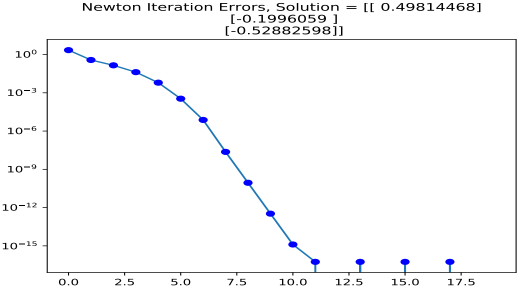
Jacobian matrix has analytic form:

$$\mathcal{J}_{\mathbf{x}}(\mathbf{F}(\mathbf{x})) = \left(\begin{array}{ccc} 3 & x_3 \sin(x_2 x_3) & x_2 \sin(x_2 x_3) \\ 2\,x_1 & -162(x_2 + 0.1) & \cos x_3 \\ -x_2\, e^{-x_1 x_2} & -x_1\, e^{-x_1 x_2} & 20 \end{array} \right).$$

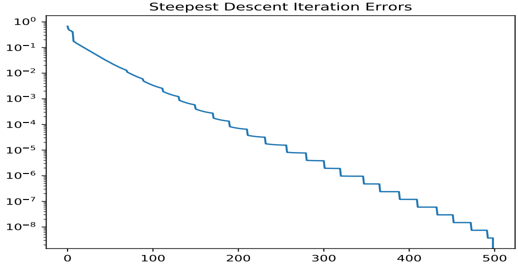
- Newton's method with $\mathbf{x}^{(0)} = (0, 0, 0)^T$



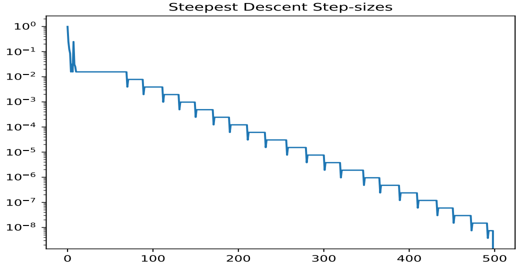
- Newton's method with $\mathbf{x}^{(0)} = -(2, 2, 2)^T$



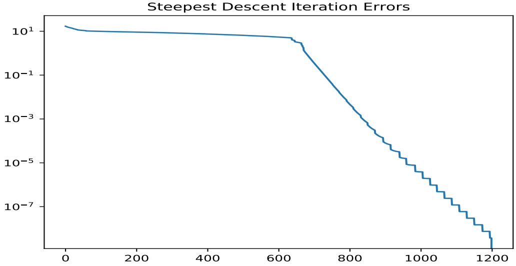
- Steepest Descent with $\mathbf{x}^{(0)} = (0, 0, 0)^T$



- Step-sizes



- Steepest Descent with $\mathbf{x}^{(0)} = -(10, 10, 10)^T$ (Newton's method diverges.)



- Step-sizes