A Different Access to Krylov Methods
Extrapolation Methods

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Iterative Methods

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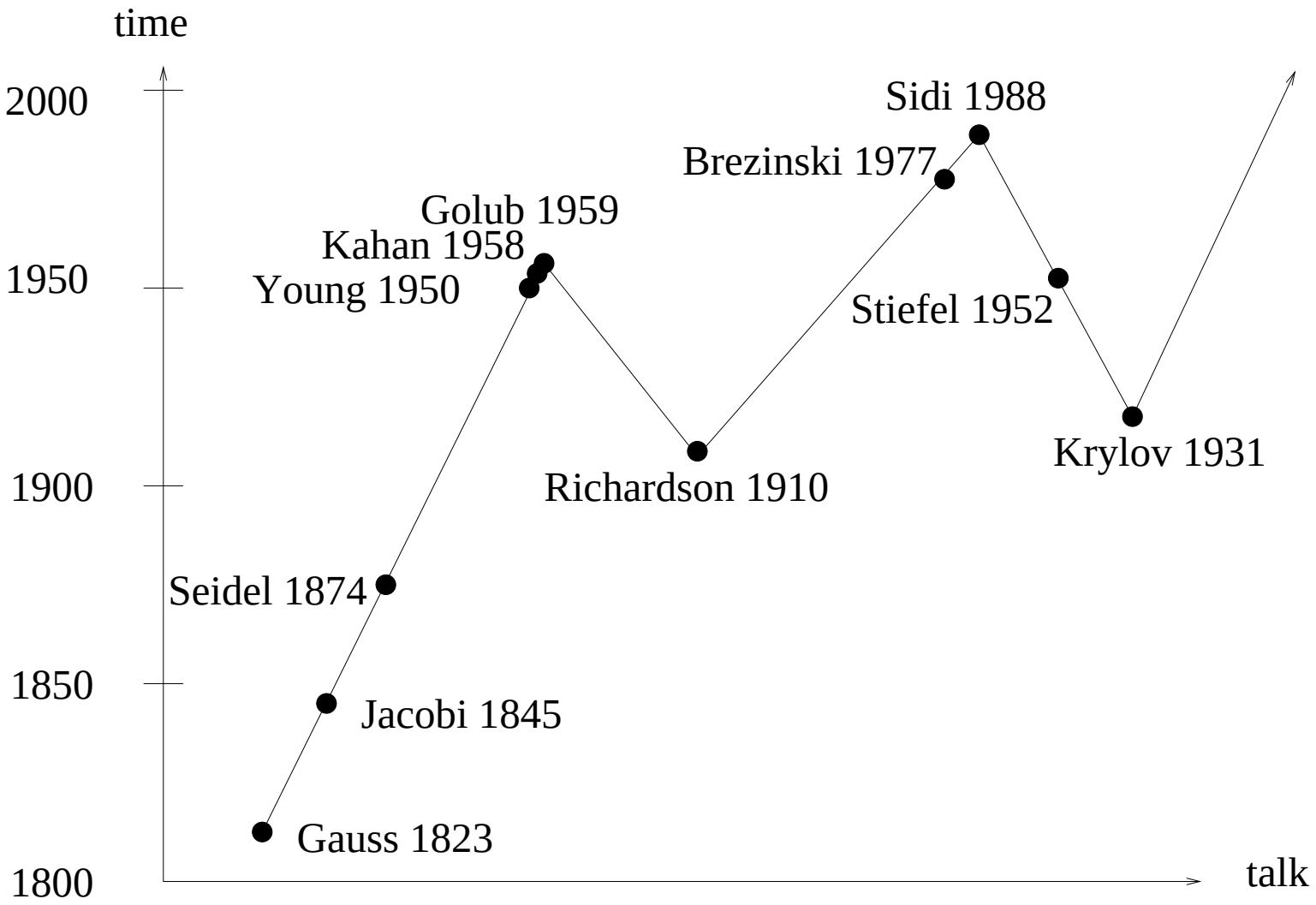

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Gauss Invents an Iterative Method in a Letter

Gauss (1823), in a letter to Gerling: in order to compute a least squares solution based on angle measurements between the locations Berger Warte, Johannisberg, Taufstein and Milseburg:

Die Bedingungsgleichungen sind also:

$$
\begin{aligned}
0 &= +\quad 6 + 67a - 13b - 28c - 26d \\
0 &= -\ 7558 - 13a + 69b - 50c - 6d \\
0 &= -14604 - 28a - 50b + 156c - 78d \\
0 &= +22156 - 26a - 6b - 78c + 110d;
\end{aligned}
$$

$$\text{Summe} = 0.$$

Um nun indirect zu eliminiren, bemerke ich, dass, wenn 3 der Grössen a, b, c, d gleich 0 gesetzt werden, die vierte den grössten Werth bekommt, wenn d dafür gewählt wird. Natürlich muss jede Grösse aus ihrer eigenen Gleichung, also d aus der vierten, bestimmt werden. Ich setze also $d = -201$ und substituire diesen Werth. Die absoluten Theile werden dann: $+5232$, -6352, $+1074$, $+46$; das Übrige bleibt dasselbe.

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Gauss' Method

Jetzt lasse ich b an die Reihe kommen, finde $b = +92$, substituire und finde die absoluten Theile: $+4036$, -4, -3526, -506. So fahre ich fort, bis nichts mehr zu corrigiren ist. Von dieser ganzen Rechnung schreibe ich aber in der Wirklichkeit bloss folgendes Schema:

	$d = -201$	$b = +92$	$a = -60$	$c = +12$	$a = +5$	$b = -2$	$a = -1$
$+6$	$+5232$	$+4036$	$+16$	-320	$+15$	$+41$	-26
-7558	-6352	-4	$+776$	$+176$	$+111$	-27	-14
-14604	$+1074$	-3526	-1846	$+26$	-114	-14	$+14$
$+22156$	$+46$	-506	$+1054$	$+118$	-12	0	$+26.$

Insofern ich die Rechnung nur auf das nächste 2000^{tel} [der] Secunde führe, sehe ich, dass jetzt nichts mehr zu corrigiren ist. Ich sammle daher

$a = -60$	$b = +92$	$c = +12$	$d = -201$
$+5$	-2		
-1			
-56	$+90$	$+12$	-201

Calculations Make Happy !

Gauss concludes his letter with the statement:

Fast jeden Abend mache ich eine neue Auflage des Tableaus, wo immer leicht nachzuhelfen ist. Bei der Einförmigkeit des Messungsgeschäfts gibt dies immer eine angenehme Unterhaltung; man sieht dann auch immer gleich, ob etwas zweifelhaftes eingeschlichen ist, was noch wünschenswerth bleibt, etc. Ich empfehle Ihnen diesen Modus zur Nachahmung. Schwerlich werden Sie je wieder direct eliminiren, wenigstens nicht, wenn Sie mehr als 2 Unbekannte haben. Das indirecte Verfahren lässt sich halb im Schlafe ausführen, oder man kann während desselben an andere Dinge denken.

"... You will in future hardly eliminate directly, at least not when you have more than two unknowns. The indirect procedure can be done while one is half asleep, or is thinking about other things."

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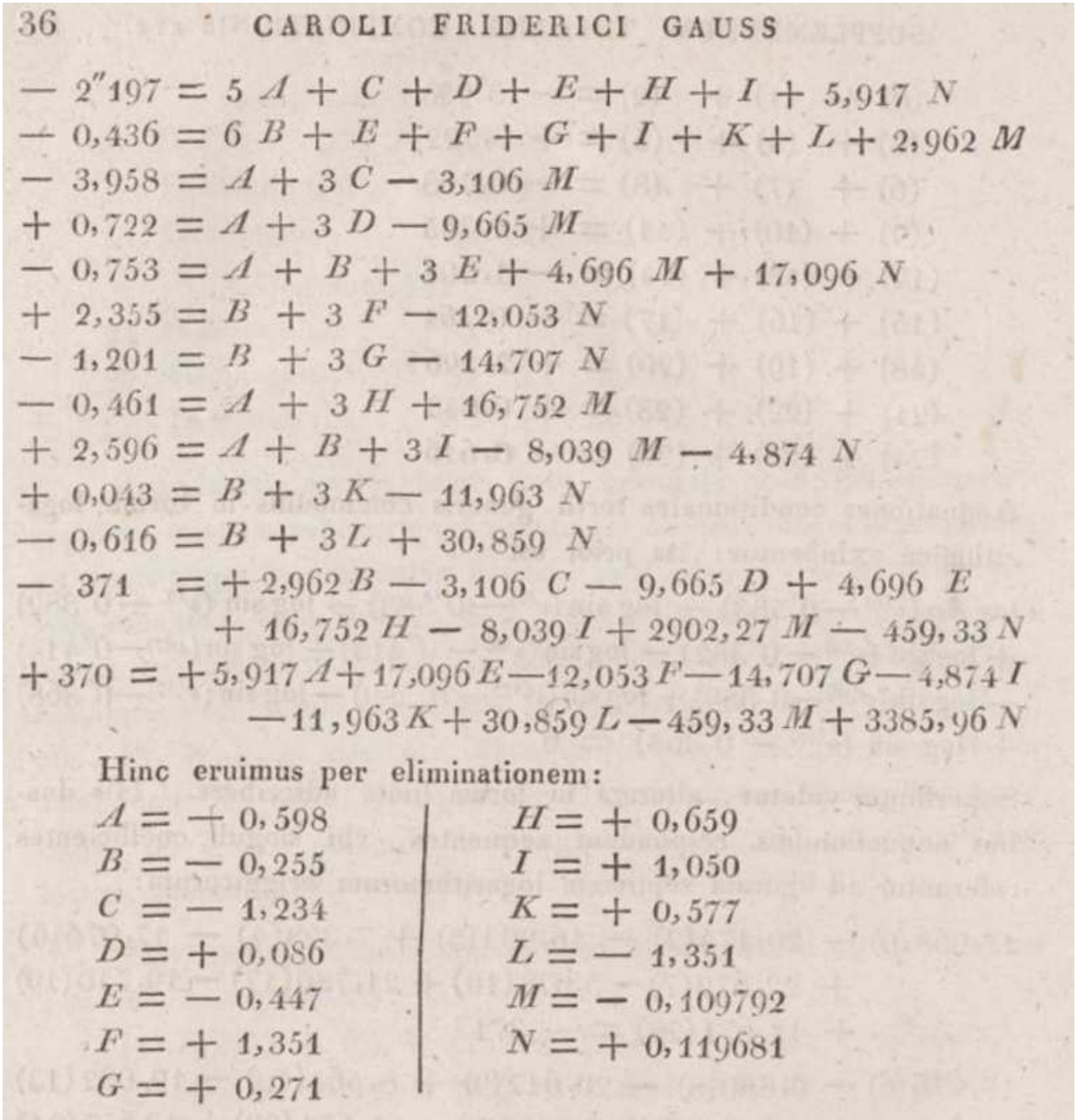
Supp. Theoria Combinationis Observationum 1828



36 CAROLI FRIDERICI GAUSS

$$
\begin{aligned}
-2''197 &= 5A + C + D + E + H + I + 5{,}917\,N \\
-0{,}436 &= 6B + E + F + G + I + K + L + 2{,}962\,M \\
-3{,}958 &= A + 3C - 3{,}106\,M \\
+0{,}722 &= A + 3D - 9{,}665\,M \\
-0{,}753 &= A + B + 3E + 4{,}696\,M + 17{,}096\,N \\
+2{,}355 &= B + 3F - 12{,}053\,N \\
-1{,}201 &= B + 3G - 14{,}707\,N \\
-0{,}461 &= A + 3H + 16{,}752\,M \\
+2{,}596 &= A + B + 3I - 8{,}039\,M - 4{,}874\,N \\
+0{,}043 &= B + 3K - 11{,}963\,N \\
-0{,}616 &= B + 3L + 30{,}859\,N \\
-371 &= +2{,}962\,B - 3{,}106\,C - 9{,}665\,D + 4{,}696\,E \\
&\quad + 16{,}752\,H - 8{,}039\,I + 2902{,}27\,M - 459{,}33\,N \\
+370 &= +5{,}917\,A + 17{,}096\,E - 12{,}053\,F - 14{,}707\,G - 4{,}874\,I \\
&\quad - 11{,}963\,K + 30{,}859\,L - 459{,}33\,M + 3385{,}96\,N
\end{aligned}
$$

Hinc eruimus per eliminationem:

$A = -0{,}598$	$H = +0{,}659$
$B = -0{,}255$	$I = +1{,}050$
$C = -1{,}234$	$K = +0{,}577$
$D = +0{,}086$	$L = -1{,}351$
$E = -0{,}447$	$M = -0{,}109792$
$F = +1{,}351$	$N = +0{,}119681$
$G = +0{,}271$	

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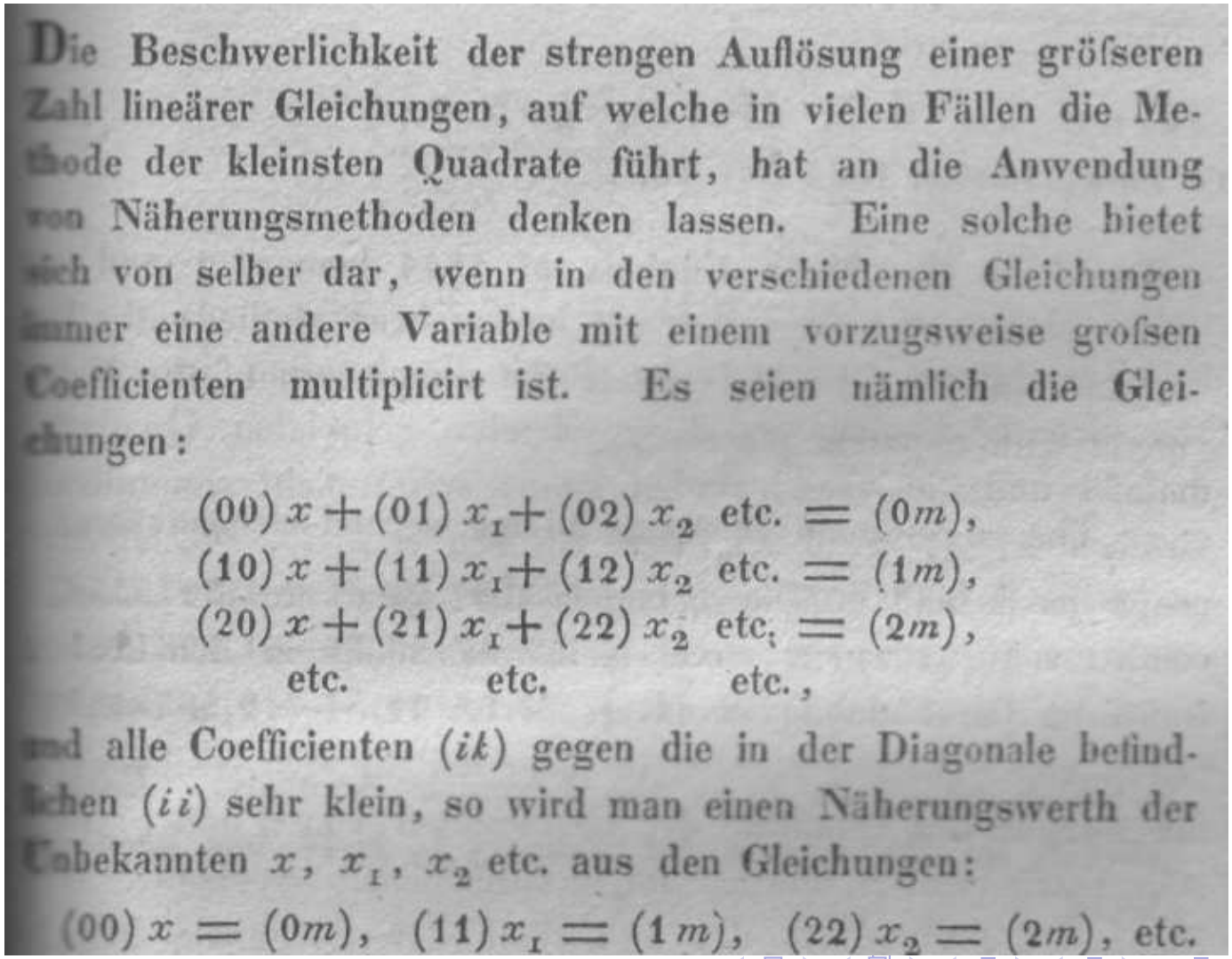
Jacobi also Invents an Iterative Method

Jacobi (1845): Ueber eine neue Auflösungsart der bei der Methode der kleinsten Quadrate vorkommenden lineären Gleichungen



Die Beschwerlichkeit der strengen Auflösung einer gröfseren Zahl lineärer Gleichungen, auf welche in vielen Fällen die Methode der kleinsten Quadrate führt, hat an die Anwendung von Näherungsmethoden denken lassen. Eine solche bietet sich von selber dar, wenn in den verschiedenen Gleichungen immer eine andere Variable mit einem vorzugsweise grofsen Coefficienten multiplicirt ist. Es seien nämlich die Gleichungen:

$$\begin{aligned}
(00)\,x + (01)\,x_1 + (02)\,x_2 \text{ etc.} &= (0m),\\
(10)\,x + (11)\,x_1 + (12)\,x_2 \text{ etc.} &= (1m),\\
(20)\,x + (21)\,x_1 + (22)\,x_2 \text{ etc.} &= (2m),\\
\text{etc.} \quad \text{etc.} \quad \text{etc.},&
\end{aligned}$$

und alle Coefficienten (ik) gegen die in der Diagonale befindlichen (ii) sehr klein, so wird man einen Näherungswerth der Unbekannten x, x_1, x_2 etc. aus den Gleichungen:

$$(00)\,x = (0m), \quad (11)\,x_1 = (1m), \quad (22)\,x_2 = (2m), \text{ etc.}$$

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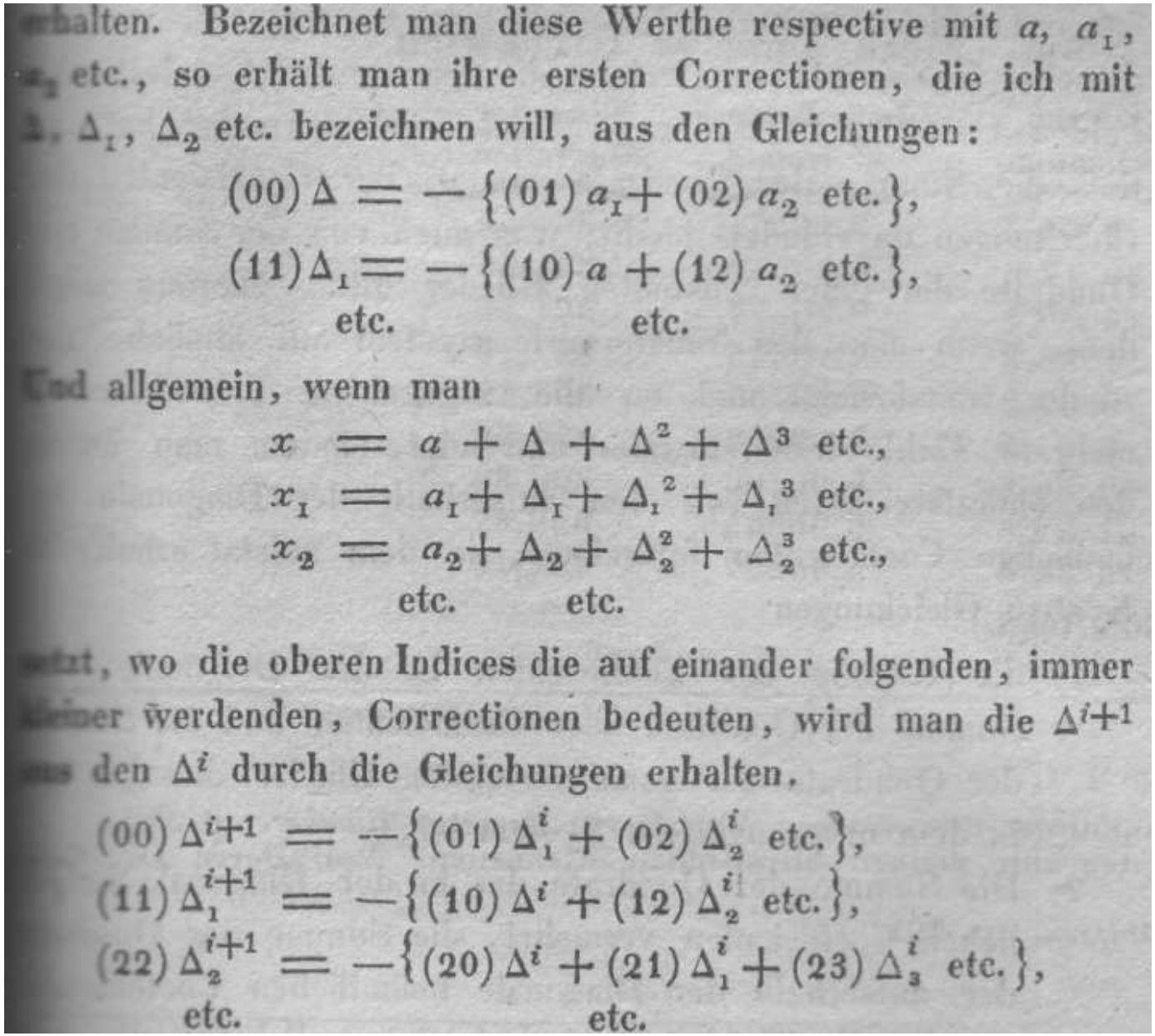
Jacobi's Method



erhalten. Bezeichnet man diese Werthe respective mit a, a_1, a_2 etc., so erhält man ihre ersten Correctionen, die ich mit Δ, Δ_1, Δ_2 etc. bezeichnen will, aus den Gleichungen:

$$(00)\,\Delta = -\{(01)\,a_1 + (02)\,a_2 \text{ etc.}\},$$
$$(11)\,\Delta_1 = -\{(10)\,a + (12)\,a_2 \text{ etc.}\},$$
$$\text{etc.} \qquad \text{etc.}$$

Und allgemein, wenn man

$$x = a + \Delta + \Delta^2 + \Delta^3 \text{ etc.},$$
$$x_1 = a_1 + \Delta_1 + \Delta_1^2 + \Delta_1^3 \text{ etc.},$$
$$x_2 = a_2 + \Delta_2 + \Delta_2^2 + \Delta_2^3 \text{ etc.},$$
$$\text{etc.} \qquad \text{etc.}$$

setzt, wo die oberen Indices die auf einander folgenden, immer kleiner werdenden, Correctionen bedeuten, wird man die Δ^{i+1} aus den Δ^i durch die Gleichungen erhalten.

$$(00)\,\Delta^{i+1} = -\{(01)\,\Delta_1^i + (02)\,\Delta_2^i \text{ etc.}\},$$
$$(11)\,\Delta_1^{i+1} = -\{(10)\,\Delta^i + (12)\,\Delta_2^i \text{ etc.}\},$$
$$(22)\,\Delta_2^{i+1} = -\{(20)\,\Delta^i + (21)\,\Delta_1^i + (23)\,\Delta_3^i \text{ etc.}\},$$
$$\text{etc.} \qquad \text{etc.}$$

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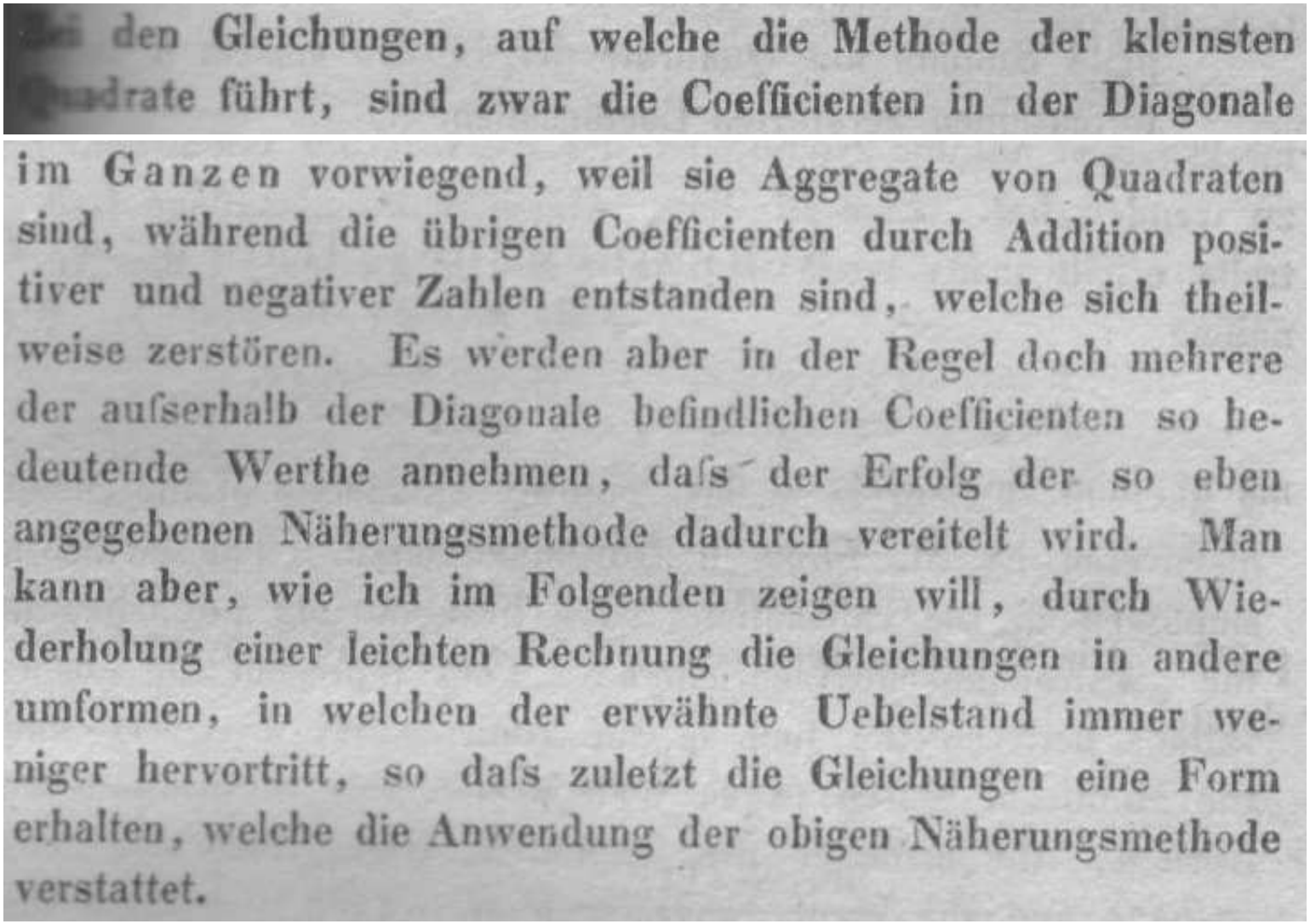
New Idea of Jacobi



den Gleichungen, auf welche die Methode der kleinsten
drate führt, sind zwar die Coefficienten in der Diagonale
im Ganzen vorwiegend, weil sie Aggregate von Quadraten
sind, während die übrigen Coefficienten durch Addition posi-
tiver und negativer Zahlen entstanden sind, welche sich theil-
weise zerstören. Es werden aber in der Regel doch mehrere
der aufserhalb der Diagonale befindlichen Coefficienten so be-
deutende Werthe annehmen, dafs der Erfolg der so eben
angegebenen Näherungsmethode dadurch vereitelt wird. Man
kann aber, wie ich im Folgenden zeigen will, durch Wie-
derholung einer leichten Rechnung die Gleichungen in andere
umformen, in welchen der erwähnte Uebelstand immer we-
niger hervortritt, so dafs zuletzt die Gleichungen eine Form
erhalten, welche die Anwendung der obigen Näherungsmethode
verstattet.

. . . and he invents the Jacobi rotations !

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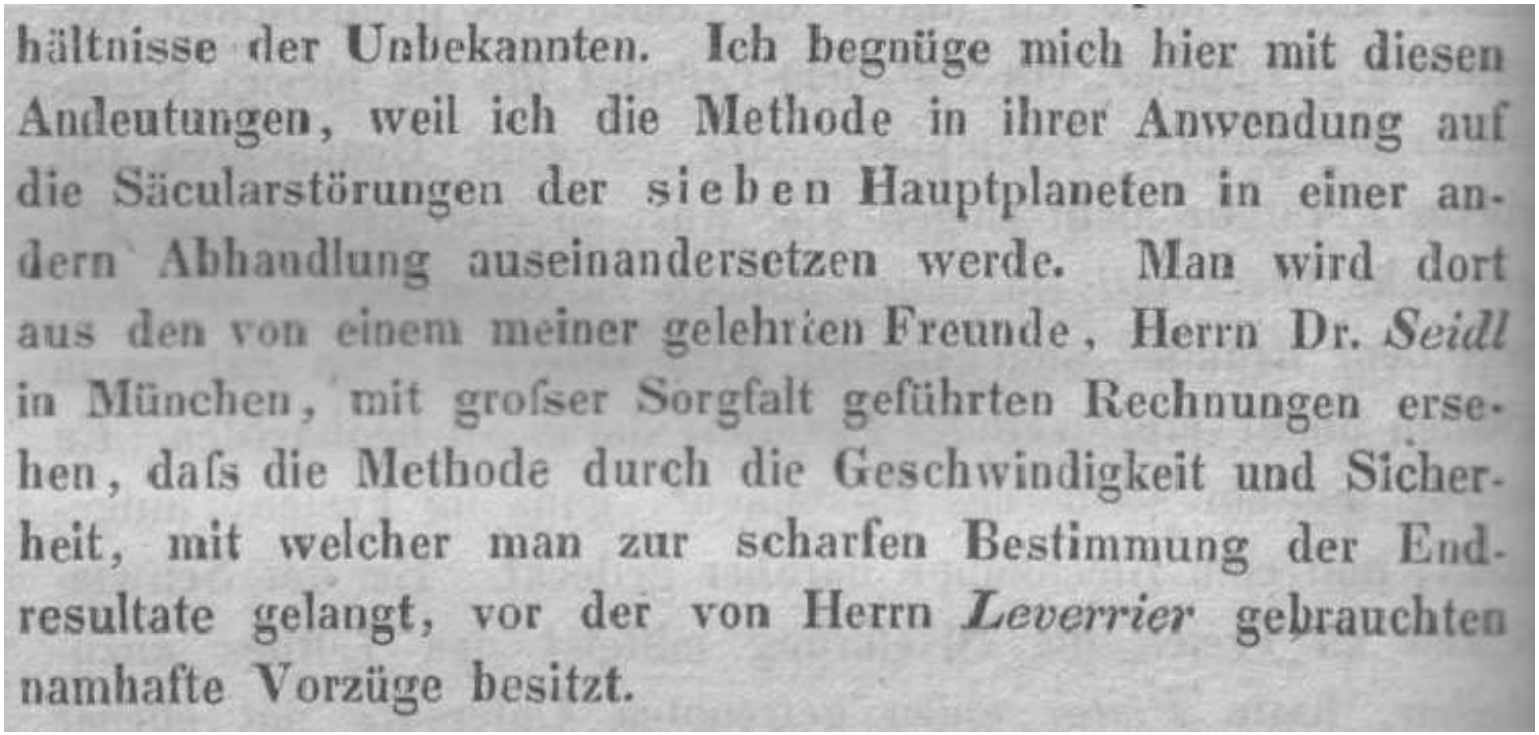

hältnisse der Unbekannten. Ich begnüge mich hier mit diesen Andeutungen, weil ich die Methode in ihrer Anwendung auf die Säcularstörungen der sieben Hauptplaneten in einer andern Abhandlung auseinandersetzen werde. Man wird dort aus den von einem meiner gelehrten Freunde, Herrn Dr. *Seidl* in München, mit grofser Sorgfalt geführten Rechnungen ersehen, dafs die Methode durch die Geschwindigkeit und Sicherheit, mit welcher man zur scharfen Bestimmung der Endresultate gelangt, vor der von Herrn *Leverrier* gebrauchten namhafte Vorzüge besitzt.

Next, Jacobi takes an example from Gauss' Theoria Motus Corporum Coelestium in Sectionibus Conicis Solem Ambientium (1809)

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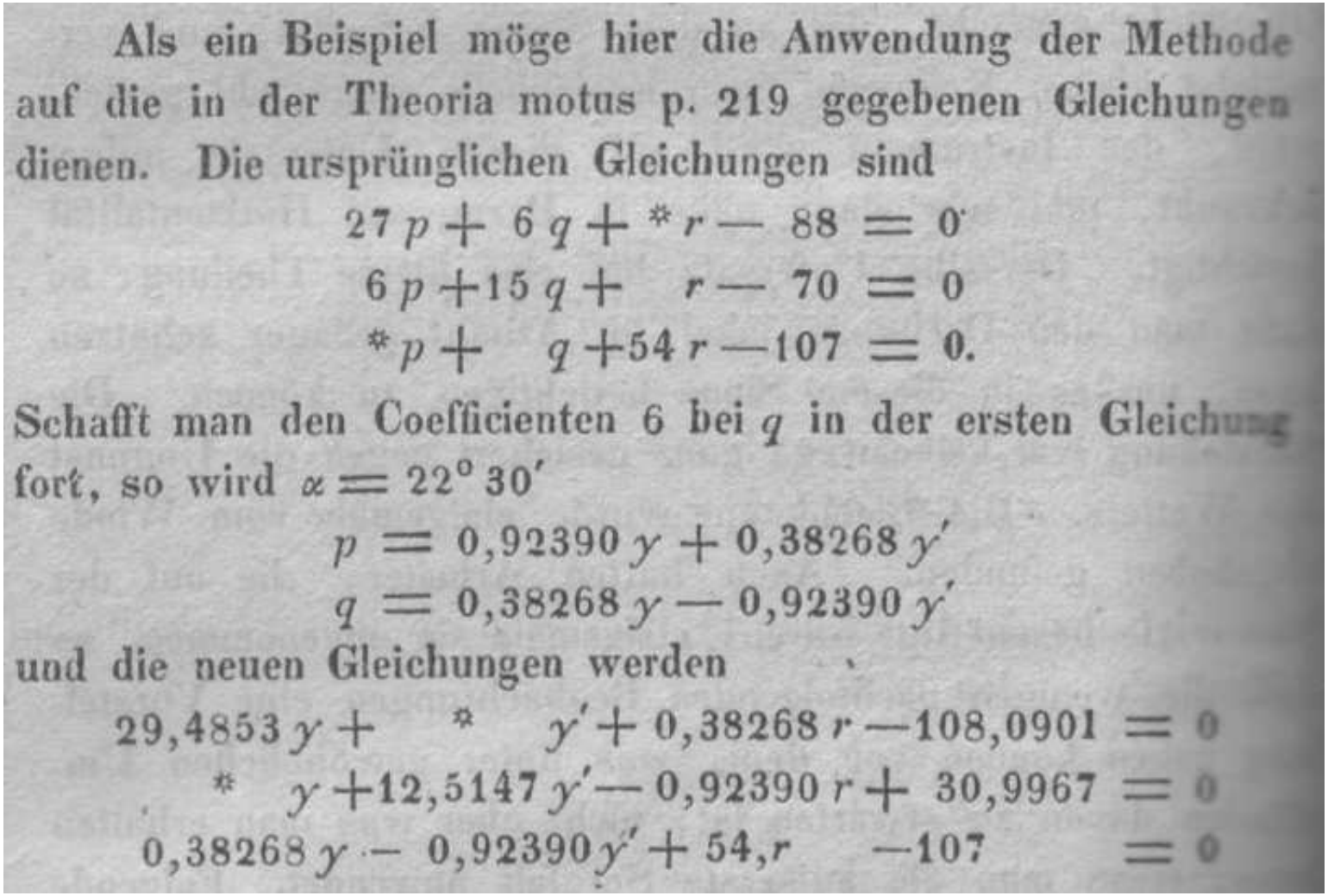
Jacobi does Preconditioning



Als ein Beispiel möge hier die Anwendung der Methode auf die in der Theoria motus p. 219 gegebenen Gleichungen dienen. Die ursprünglichen Gleichungen sind

$$\begin{aligned} 27p + 6q + *r - 88 &= 0 \\ 6p + 15q + r - 70 &= 0 \\ *p + q + 54r - 107 &= 0. \end{aligned}$$

Schafft man den Coefficienten 6 bei q in der ersten Gleichung fort, so wird $\alpha = 22^\circ 30'$

$$\begin{aligned} p &= 0{,}92390\,y + 0{,}38268\,y' \\ q &= 0{,}38268\,y - 0{,}92390\,y' \end{aligned}$$

und die neuen Gleichungen werden

$$\begin{aligned} 29{,}4853\,y + * y' + 0{,}38268\,r - 108{,}0901 &= 0 \\ * y + 12{,}5147\,y' - 0{,}92390\,r + 30{,}9967 &= 0 \\ 0{,}38268\,y - 0{,}92390\,y' + 54{,}r - 107 &= 0 \end{aligned}$$

After preconditioning, it takes only three Jacobi iterations to obtain three accurate digits!

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Ludwig Seidel

Seidel (1874): Ueber ein Verfahren, die Gleichungen, auf welche die Methode der kleinsten Quadrate führt, sowie lineäre Gleichungen ueberhaupt, durch successive Annäherung aufzulösen

So einfach nun, ihrer mathematischen Natur nach, die Aufgabe ist, eine beliebige Anzahl unbekannter Grössen aus gleich vielen linearen Gleichungen zu berechnen, so mühsam wird ihre numerische Durchführung, wenn die Zahl der Unbekannten beträchtlich gross wird,

der anzuschliessen. Ich weiss nicht, ob ein Complex von mehr als einigen siebzig Unbekannten je einheitlich berechnet worden ist. Die Zahl 70 ist erreicht in dem Netze der ostpreussischen Gradmessung[1]) (und zwar in einem Falle, wo zwischen den Unbekannten noch 31 streng zu erfüllende Bedingungsgleichungen bestehen, welcher Umstand aber nach der gewöhnlichen Art der Behandlung die Sache nur erschwert), und mit 72 Unbekannten habe ich zu thun gehabt bei Berechnung der wahrscheinlichsten Werthe für die Logarithmen der Helligkeiten der Sterne, welche in mein photometrisches Netz gezogen waren[2]) — Die gebräuch-

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Seidel was Jacobi's Student

Seidel talks about Jacobi, and how he had the honor to calculate for him:

Ein anderes Verfahren hat Jacobi erdacht und auf die 7 Gleichungen angewandt, welche zur Berechnung eines Theiles der Säcularstörungen im Planetensystem nach Laplace von Leverrier aufgestellt waren[1]); ich habe noch als Studirender die Ehre gehabt, für ihn dazu die numerischen Rechnungen auszuführen.

but he also did not think much about the preconditioning idea of Jacobi:

So sinnreich übrigens diese Methode den speciellen Schwierigkeiten des Falles angepasst ist, für welchem Jacobi ihre Anwendung veranlasste und in welchem die diagonalen Coefficienten selbst noch lineäre Funktionen einer supernumerären Unbekannten sind, so scheint sie mir für den gewöhnlich vorkommenden einfacheren Fall doch keineswegs vortheilhafter zu sein, als die allgemein angewandte; auch bezweifle ich, ob sie in irgend einem weiteren Falle bisher in Anwendung gebracht worden ist.

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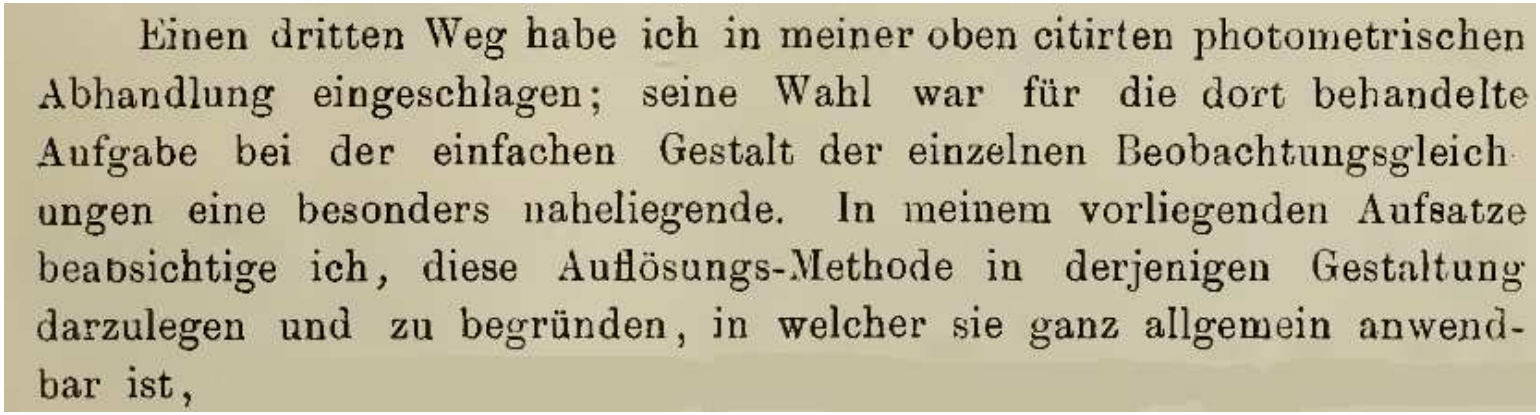
Seidel's "New Method"

Seidel then proposes a third method, his method:



Einen dritten Weg habe ich in meiner oben citirten photometrischen Abhandlung eingeschlagen; seine Wahl war für die dort behandelte Aufgabe bei der einfachen Gestalt der einzelnen Beobachtungsgleichungen eine besonders naheliegende. In meinem vorliegenden Aufsatze beabsichtige ich, diese Auflösungs-Methode in derjenigen Gestaltung darzulegen und zu begründen, in welcher sie ganz allgemein anwendbar ist,

- Seidel describes in what follows Gauss' method
- He gives a convergence prove for the case of the normal equations
- He emphasizes that any system can be written as a system of normal equations
- He notes that the unknowns could also be processed cyclically
- and ...

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Seidel Does Parallel Computing!

Verbindung gebracht werden sollen; d. h. man nehme an, dass das Beobachtungsmaterial (niedergelegt in Gleichungen der Form A), welches sehr viele Unbekannte enthalten mag, sich unter zwei Rechner so vertheilen lässt, dass die Gleichungen, welche gewisse Unbekannte enthalten, ausschliesslich dem ersten, diejenigen mit anderen Unbekannten ausschliesslich dem zweiten zugewiesen werden, und dass nur verhältnissmässig wenig Unbekannte einer dritten oder intermediären Gruppe durch Beobachtungsgleichungen einerseits mit Variablen des ersten und andererseits mit solchen des zweiten Systemes in Verbindung gebracht sind, und so den Zusammenhang beider Systeme vermitteln. Die Normalgleichungen (in der Form E, E') für die Unbekannten dieser verbindenden Art müssen von beiden Rechnern (natürlich übereinstimmend) angesetzt werden: ihre Glieder zur Rechten (auch die Complexe $\xi . \eta \ldots$) werden von selbst in drei Theile zerfallen, die Unbekannten des ersten, des zweiten und des intermediären Systems, resp. deren Correctionen, enthaltend. Ausserdem hat jeder Rechner vor sich die Normalgleichungen für die ihm allein zugetheilten Unbekannten. Indem nun ausgeglichen wird, muss von Zeit zu Zeit an gewissen Abschnitten der Arbeit jeder Rechner dem andern für die Normalgleichungen der gemeinsamen Unbekannten die Zahlenwerthe derjenigen Glieder mittheilen,

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Modern Notation

Large sparse linear system

$$A\mathbf{x} = \mathbf{b}, \quad A \in \mathbb{R}^{n\times n}, \quad \mathbf{b} \in \mathbb{R}^n,$$

Split the matrix, $A = M - N$, and iterate

$$M\mathbf{x}_{k+1} = N\mathbf{x}_k + \mathbf{b}, \quad k = 0, 1, 2, \ldots$$

Stationary iterative method: M and N do not depend on k

Conditions on M:

- M is a good approximation of A,
- $M\mathbf{x} = \mathbf{y}$ is easy and cheap to solve.

Standard form: $\mathbf{x}_{k+1} = M^{-1}N\mathbf{x}_k + M^{-1}\mathbf{b}$
Correction form: $\mathbf{x}_{k+1} = \mathbf{x}_k + M^{-1}(\mathbf{b} - A\mathbf{x}_k)$

Residual, Error and the Difference of Iterates

Theorem: Defining the

- error: $\mathbf{e}_k := \mathbf{x} - \mathbf{x}_k$
- residual: $\mathbf{r}_k := \mathbf{b} - A\mathbf{x}_k$
- difference of iterates: $\mathbf{u}_k := \mathbf{x}_{k+1} - \mathbf{x}_k$

we have

$$\begin{aligned} \mathbf{e}_{k+1} &= M^{-1}N\mathbf{e}_k, \\ \mathbf{u}_{k+1} &= M^{-1}N\mathbf{u}_k, \\ \mathbf{r}_{k+1} &= NM^{-1}\mathbf{r}_k, \end{aligned}$$

and difference, error and residual are related by

$$M\mathbf{u}_k = \mathbf{r}_k = A\mathbf{e}_k.$$

Theorem (Nekrasov 1885, Pizzetti 1887) The method converges iff $\rho(M^{-1}N) < 1$.

Convergence Factor and Convergence Rate

$$\mathbf{e}_k = (M^{-1}N)^k \mathbf{e}_0 = G^k \mathbf{e}_0$$

taking norms, we want for the error reduction to tolerance ε

$$\frac{\|\mathbf{e}_k\|}{\|\mathbf{e}_0\|} \leq \|G^k\| = \left(\left\|G^k\right\|^{\frac{1}{k}}\right)^k < \varepsilon \Longrightarrow k > \frac{\ln(\varepsilon)}{\ln\left(\|G^k\|^{\frac{1}{k}}\right)}.$$

Lemma: For any induced matrix norm, we have

$$\lim_{k\to\infty} \|G^k\|^{\frac{1}{k}} = \rho(G).$$

Definition:

- mean convergence factor: $\rho_k(G) = \|G^k\|^{\frac{1}{k}}$
- asymptotic convergence factor: $\rho(G) = \lim_{k\to\infty} \rho_k(G)$
- mean convergence rate
  $R_k(G) = -\ln\left(\|G^k\|^{\frac{1}{k}}\right) = -\ln(\rho_k(G))$
- asymptotic convergence rate $R_\infty(G) = -\ln(\rho(G))$

Jacobi's Method

One step of Jacobi for the system $Ax = b$

```
for i=1:n
  tmp(i)=(b(i)-A(i,[1:i-1 i+1:n])*x([1:i-1 i+1:n]))/A(i,i);
end
x=tmp(:);
```

This corresponds to the splitting $A = M - N$ with

$$M = D, \quad N = -L - U \quad \Longrightarrow \quad D\mathbf{x}_{k+1} = \mathbf{b} - (L + U)\mathbf{x}_k$$

Theorem: If the matrix $A \in \mathbb{R}^{n\times n}$ is strictly diagonally dominant , i.e.

$$|a_{ii}| > \sum_{j\neq i} |a_{ij}| \quad \text{for } i = 1, \ldots, n,$$

then the Jacobi iteration converges.

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Gauss-Seidel

One step of Gauss-Seidel for the system $Ax = b$

```
for i=1:n
  x(i)=(b(i)-A(i,[1:i-1 i+1:n])*x([1:i-1 i+1:n]))/A(i,i);
end
```

This corresponds to the splitting

$$M = D + L, \quad N = -U$$

$$\Longrightarrow (D + L)\mathbf{x}_{k+1} = -U\mathbf{x}_k + \mathbf{b}.$$

Remark: Gauss-Seidel is often faster than Jacobi, e.g. for the Laplacian, Gauss-Seidel converges twice as fast as Jacobi

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Gauss-Seidel always faster than Jacobi ?

$$A = \begin{pmatrix} -1 & 0 & -1 \\ -1 & 1 & 0 \\ 1 & 2 & -3 \end{pmatrix}$$

The Jacobi iteration matrix

$$G_{\mathrm{J}} = -D^{-1}(L+U) = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix},$$

has eigenvalues $0.37 \pm 0.86i$ and -0.74, $\rho(G_{\mathrm{J}}) = 0.944$.
Gauss-Seidel iteration matrix

$$G_{\mathrm{GS}} = -(D+L)^{-1}U = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -1 \\ 0 & 0 & -1 \end{pmatrix},$$

has eigenvalues 0, 0, -1 with $\rho(G_{\mathrm{GS}}) = 1$.

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Successive Overrelaxation

One step of Successive Overrelaxation (Young 1950) with parameter ω for the system $Ax = b$

```
for i=1:n
  x(i)=omega*(b(i)-A(i,[1:i-1 i+1:n])*x([1:i-1 i+1:n]))/A(i,i)
       +(1-omega)*x(i);
end
```

SOR can also be derived from Gauss-Seidel

$$(D + L)\mathbf{x} = -U\mathbf{x} + \mathbf{b}.$$

Multiplying by ω and adding on both sides the expression $(1 - \omega)D\mathbf{x}$, we obtain the SOR iteration

$$(D + \omega L)\mathbf{x}_{k+1} = (-\omega U + (1 - \omega)D)\mathbf{x}_k + \omega\mathbf{b}.$$

SOR is therefore based on the splitting

$$A = M - N \text{ with } M = \frac{1}{\omega}D + L \text{ and } N = -U + \left(\frac{1}{\omega} - 1\right) D$$

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Convergence Results for SOR

Theorem [Kahan (1958)]: For the SOR iteration matrix

$$G_{\mathrm{SOR}} = (D + \omega L)^{-1}(-\omega U + (1-\omega)D)$$

we have

$$\rho(G_{\mathrm{SOR}}) \geq |\omega - 1|, \ \forall \omega.$$

Theorem [Ostrowski-Reich]: Let $A \in \mathbb{R}^{n \times n}$ be symmetric and invertible, with positive diagonal elements, $D > 0$. Then SOR converges for all $0 < \omega < 2$ if and only if A is positive definite.

Optimal Choice of Relaxation

Theorem [Young 1950]: Let A have property A, i.e. there exist diagonal matrices D_1 and D_2 s.t

$$\tilde{A} = P^T A P = \begin{bmatrix} D_1 & F \\ E & D_2 \end{bmatrix} = L + D + U.$$

Let $G_{\mathrm{J}}(\tilde{A})$ be the associated Jacobi iteration matrix. If the eigenvalues $\mu(G_{\mathrm{J}})$ are real and $\rho(G_{\mathrm{J}}) < 1$, then the optimal SOR parameter ω for $\tilde{A}$ is

$$\omega_{\mathrm{opt}} = \frac{2}{1 + \sqrt{1 - \rho(G_{\mathrm{J}})^2}}.$$

Example: For the discretized Laplacian, Jacobi and Gauss-Seidel have convergence factors $1 - O(h^2)$, and optimized SOR has a convergence factor $1 - O(h)$.

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Richardson Iteration

From the correction form of the stationary iteration

$$\mathbf{x}_{k+1} = \mathbf{x}_k + M^{-1}\mathbf{r}_k,$$

choosing $M^{-1} = \alpha I$, which corresponds to the splitting $M = \frac{1}{\alpha} I$ and $N = \frac{1}{\alpha} I - A$, leads to Richardson's method

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha(\mathbf{b} - A\mathbf{x}_k) = (I - \alpha A)\mathbf{x}_k + \alpha\mathbf{b}.$$

Theorem: For $A \in \mathbb{R}^{n\times n}$ symmetric and positive definite:

a) Richardson converges $\iff$ $0 < \alpha < \frac{2}{\rho(A)}$.

b) Convergence is optimal for $\alpha_{\text{opt}} = \frac{2}{\lambda_{\max}(A)+\lambda_{\min}(A)}$.

c) $\rho(I - \alpha_{\text{opt}} A) = \frac{\kappa(A)-1}{\kappa(A)+1}$, $\kappa(A) := \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$.

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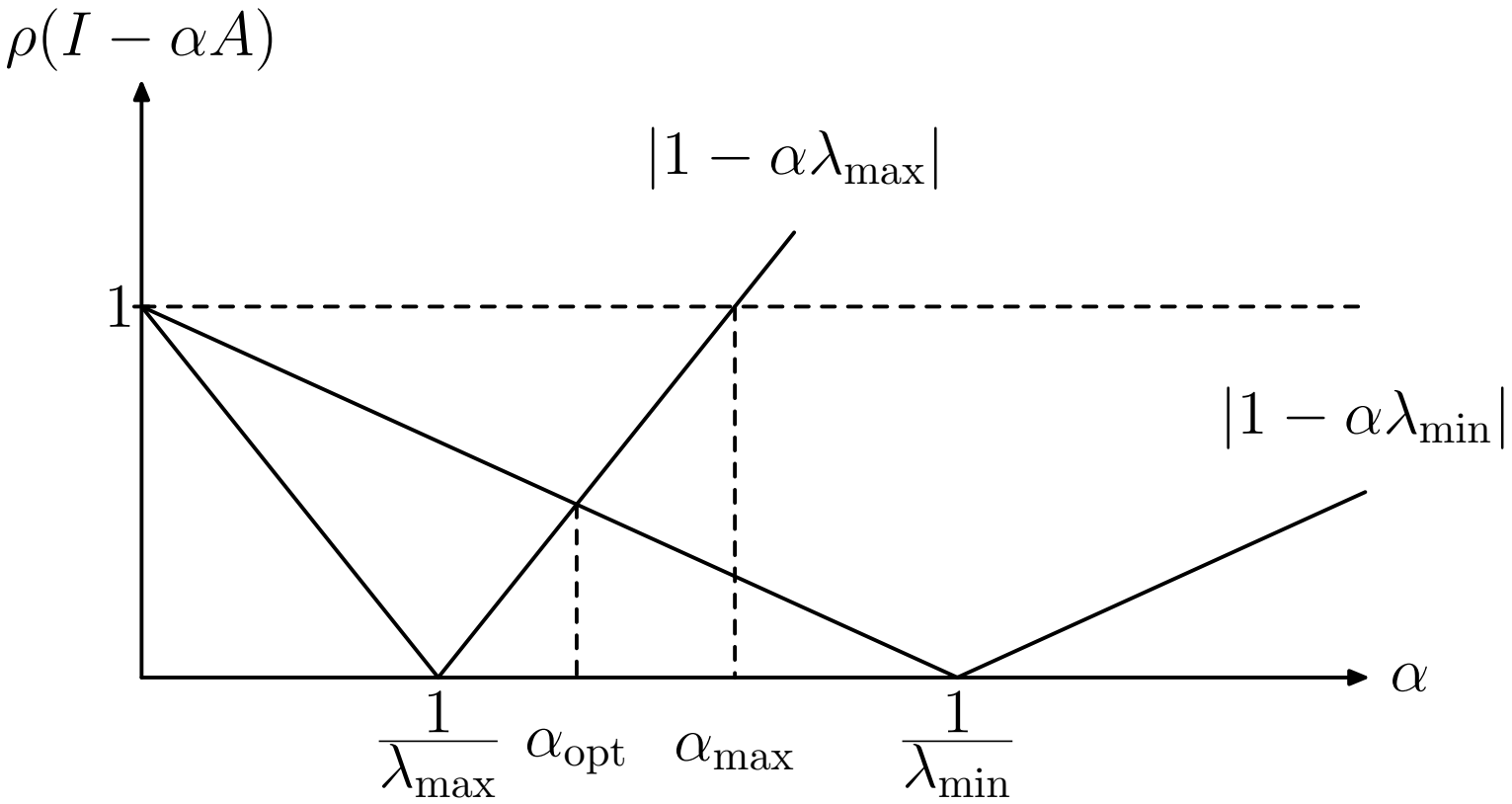
Proof of the Theorem



Remark: For the Laplacian, we get the convergence factor $1 - O(h^2)$

But is this really what Richardson proposed ???

Richardson's Influential Paper

Richardson (1910): The Approximate Arithmetical Solution by Finite Differences of Physical Problems involving Differential Equations, with an Application to the stresses in a Masonry Dam

Contains historical section:

§ 2·0. *Historical.*—Step-by-step arithmetical methods of solving ordinary difference equations have long been employed for the calculation of interest and annuities. Recently their application to differential equations has been very greatly improved by the introduction of rules allied to those for approximate quadrature. The papers referred to are :—

RUNGE, "Über die numerische Auflösung von Differentialgleichungen," 'Math. Ann.,' Bd. 46. Leipzig, 1895.

W. F. SHEPPARD, "A Method for Extending the Accuracy of Mathematical Tables," 'Proc. Lond. Math. Soc.,' XXXI.

KARL HEUN, "Neue methode zur approximativen Integration der Differentialgleichungen einer unabhängigen Veränderlichen," 'Zeitschrift Math. u. Phys.,' No. 45, 1900.

WILHELM KUTTA, "Beitrag zur näherungsweisen Integration totaler Differentialgleichen," 'Zeitschrift Math. u. Phys.,' No. 46, 1901.

Further RICHARD GANZ, in a paper "Über die numerische Auflösung von partiellen Differentialgleichungen," 'Zeitschrift Math. u. Phys.,' No. 48, 1903, has extended the methods of RUNGE, HEUN, and KUTTA to partial equations of the type considered in this section.

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A Very Rich and Well Written Paper

Focus is the numerical solution of PDEs:

The equations considered in any detail are only a few of the commoner ones occurring in physical mathematics, namely:—LAPLACE's equation $\nabla^2\phi = 0$; the oscillation equations $(\nabla^2+k^2)\,\phi = 0$ and $(\nabla^4-k^4)\,\phi = 0$; and the equation $\nabla^4\phi = 0$. But the methods employed are not limited to these equations.

Explains finite difference approximations:

differencing operator δ and SHEPPARD's* averager μ are defined by

$$\delta f(x) = f(x+\tfrac{1}{2}h) - f(x-\tfrac{1}{2}h) \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (1),$$

$$\mu f(x) = f(x+\tfrac{1}{2}h) + f(x-\tfrac{1}{2}h) \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (2),$$

$\frac{\partial\phi}{\partial x}$ will be represented by $\mu\,\frac{\delta\phi}{\delta x} = \frac{1}{2h}\{(10)-(\bar{1}0)\}$

$\frac{\partial^2\phi}{\partial x^2}$,, ,, ,, $\frac{\delta^2\phi}{\delta x^2} = \frac{1}{h^2}\{(10)-2(00)+(\bar{1}0)\}$

$\frac{\partial^3\phi}{\partial x^3}$,, ,, ,, $\mu\,\frac{\delta^3\phi}{\delta x^3} = \frac{1}{2h^3}\{(20)-2(10)+2(\bar{1}0)-(\bar{2}0)\}$

$\frac{\partial^4\phi}{\partial x^4}$,, ,, ,, $\frac{\delta^4\phi}{\delta x^4} = \frac{1}{h^4}\{(20)-4(10)+6(00)-4(\bar{1}0)+(\bar{2}0)\}$

$\frac{\partial^2\phi}{\partial x\,\partial y}$,, ,, ,, $\mu^2\,\frac{\delta^2\phi}{\delta x\,\delta y} = \frac{1}{4h^2}\{(11)+(\bar{1}\bar{1})-(\bar{1}1)-(1\bar{1})\}$

$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}$,, ,, ,, $\frac{\delta^2\phi}{\delta x^2}+\frac{\delta^2\phi}{\delta y^2} = \nabla_1^{\,2}\phi = \frac{1}{h^2}\{(10)+(01)+(\bar{1}0)+(0\bar{1})-4(00)\}.$

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Time Stepping Methods for Evolution Problems

One of Richardson's examples: the heat equation

$$u_t = u_{xx} \quad \text{in } \Omega = (-0.5, 0.5) \times (0, 0.005)$$

TABLE I.

	$t = 0.$	0·001.	0·002.	0·003.	0·004.	0·005.	0·005 correct by FOURIER'S method.	Errors.
$x = 0·5$	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	
0·4	1·0000	$a = 0·9090$	0·8356	0·7714	0·7209	0·6729	0·6828	−0·0099
0·3	1·0000	$b = 0·9959$	0·9834	0·9695	0·9492	0·9329	0·9545	−0·0216
0·2	1·0000	$c = 0·9998$	0·9993	0·9968	0·9945	0·9887	0·9980	−0·0093
0·1	1·0000	$d = 1·0000$	1·0000	0·9999	0·9994	0·9990	0·9996	−0·0006
0·0	1·0000	$e = 1·0000$	1·0000	1·0000	1·0000	0·9998	1·0000	−0·0002
−0·1	1·0000	$d = 1·0000$	1·0000	0·9999	0·9994	0·9990	0·9996	−0·0006

In satisfying the equation we must be careful to equate values of $\partial^2\phi/\partial x^2$ and $\partial\phi/\partial t$, which are centered at the same point. This causes a little difficulty at starting. When $t = 0·001$ let the values of ϕ be a, b, c, d, e, as indicated in Table I. Then if the difference equation be satisfied at $t = 0·0005$, it takes the form of 5 simultaneous equations involving a, b, c, d, e. Solving these equations, we find the numbers given in the column $x = 0·001$. Having got over this rather troublesome first step, we can find the rest much more simply by centering all differences on the columns $t = 0·001$, 0·002, 0·003, &c., and deducing each number from the two preceding columns. The

Explains Richardson extrapolation

An excellent illustration is afforded by Lord RAYLEIGH's account of the vibration of a stretched string of beads ('Sound,' vol. I., § 121). He gives the frequency of the fundamental for the same mass per unit length concentrated in various numbers of beads. This is reproduced below in the table. The co-ordinate difference h is inversely as one plus the number of beads, not counting beads at the fixed ends.

Number of free beads + one . .	2	3	4	5	10	20	40	∞
Ratio of frequency to that of continuous string	·9003	·9549	·9745	·9836	·9959	·9990	·9997	unity
Error in representation of continuous string by string of beads	·0997	·0451	·0255	·0164	·0041	·0010	·0003	·0000
Ratio of error to square of co-ordinate difference × a constant	·3988	·4059	·4080	·4091	·4107	·4111	·4112	·4112

The degree of constancy of the last line shows that if we found the frequency for one bead and for three, then extrapolation, on the assumption that the error is proportional to h^2, would give us the frequency for the continuous string to about one part in 1000; which is as near as we could get by twenty beads and no extrapolation.

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Solution of Laplace's Equation

TABLE III.

0·5	1	1	1	1	← edge of square.
0	0·5	a	b	c	b
0		0·5	d	e	d
0			0·5	f	0·5
0				centre of 0·5 square.	

↑ edge of square.

TABLE II.

	ψ_1	β_1
ψ_3	ψ_2	β_2
β_4	β_3	

Wall Clock Times of Richardson

The solution of these six simultaneous equations was accomplished in an hour and gave the following results :—

	a.	*b.*	*c.*	*d.*	*e.*	*f.*
By finite differences	0·693	0·772	0·794	0·601	0·6324	0·533
By infinitesimals	0·700	0·777	0·798	0·604	0·6354	0·534
Errors due to finite differences . .	0·007	0·005	0·004	0·003	0·003	0·001

The numbers for infinitesimal differences were obtained from

$$\phi = \frac{4}{\pi} \sum_{m \text{ odd}} (-1)^{\frac{m-1}{2}} \frac{1}{m} \operatorname{sech} \frac{m\pi}{2} \cos mx \cosh mz,$$

"... adding up the series at these six points took 3 hours !"

Richardson also does clamped vibration, on a diamond (comparison with Rayleigh's bound, Ritz is missing!)

Richardson's Iterative Method

§ 3·2. *Successive Approximation to the Integrals.*—Having illustrated the use of simultaneous integral equations, let us pass on to methods which have this property in common: that starting from a table of numbers, correct at the boundary, but otherwise merely as near as one can guess, one proceeds by definite methods to modify this table and thereby to cause it to approach without limit towards the true finite-difference integral.

Conditions of Applicability according to Richardson:

- $\mathcal{D}\phi = 0$, $\mathcal{D}$ a differential operator, together with boundary conditions to make the problem determinate
- Equations must be linear
- Must be such that a certain positive quadratic function is a complete minimum

Let ϕ_u be the correct finite-difference integral. Let ϕ_1 be a function (that is a table of numbers) satisfying the correct boundary-conditions, but arbitrary as to its body values. Next calculate the body-values of ϕ_2 by means of

$$\phi_2 = \phi_1 - \alpha_1^{-1}\,\mathfrak{D}'\phi_1 \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (1)$$

where α_1 is a number to be fixed; and fill in such boundary-values of ϕ_2 as will satisfy the same boundary-conditions as ϕ_u. The succeeding steps are each of the form

$$\phi_{m+1} = \phi_m - \alpha_m^{-1}\,\mathfrak{D}'\phi_m \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (2)$$

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Richardson's Analysis

that by the judicious choice of $\alpha_1, \alpha_2, \ldots, \alpha_t$ it is possible to make ϕ_{t+1} nearer to ϕ_u than ϕ_1 was. For since $\mathfrak{D}'$ is linear and $\mathfrak{D}'\phi_u = 0$ we have from (2)

$$\phi_{m+1} - \phi_u = \phi_m - \phi_u - \alpha_m^{-1}\,\mathfrak{D}'\,(\phi_m - \phi_u). \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (3).$$

Now it is shown in the Appendix that $\phi_m - \phi_u$ may be expanded in a series of integrals of

$$(\mathfrak{D}' - \lambda_k^2)\,\mathrm{P}_k = 0 \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (4).$$

Put $$\phi_1 - \phi_u = \Sigma \mathrm{A}_k \mathrm{P}_k \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (5).$$

Then by (4) $$\mathfrak{D}'\,(\phi_1 - \phi_u) = +\Sigma \mathrm{A}_k \lambda_k^2 \mathrm{P}_k.$$

And therefore by (3) $$\phi_2 - \phi_u = \Sigma \mathrm{A}_k \left(1 - \frac{\lambda_k^2}{\alpha_1}\right) \mathrm{P}_k \,. \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (6).$$

Proceeding in the same manner after t operations we arrive at

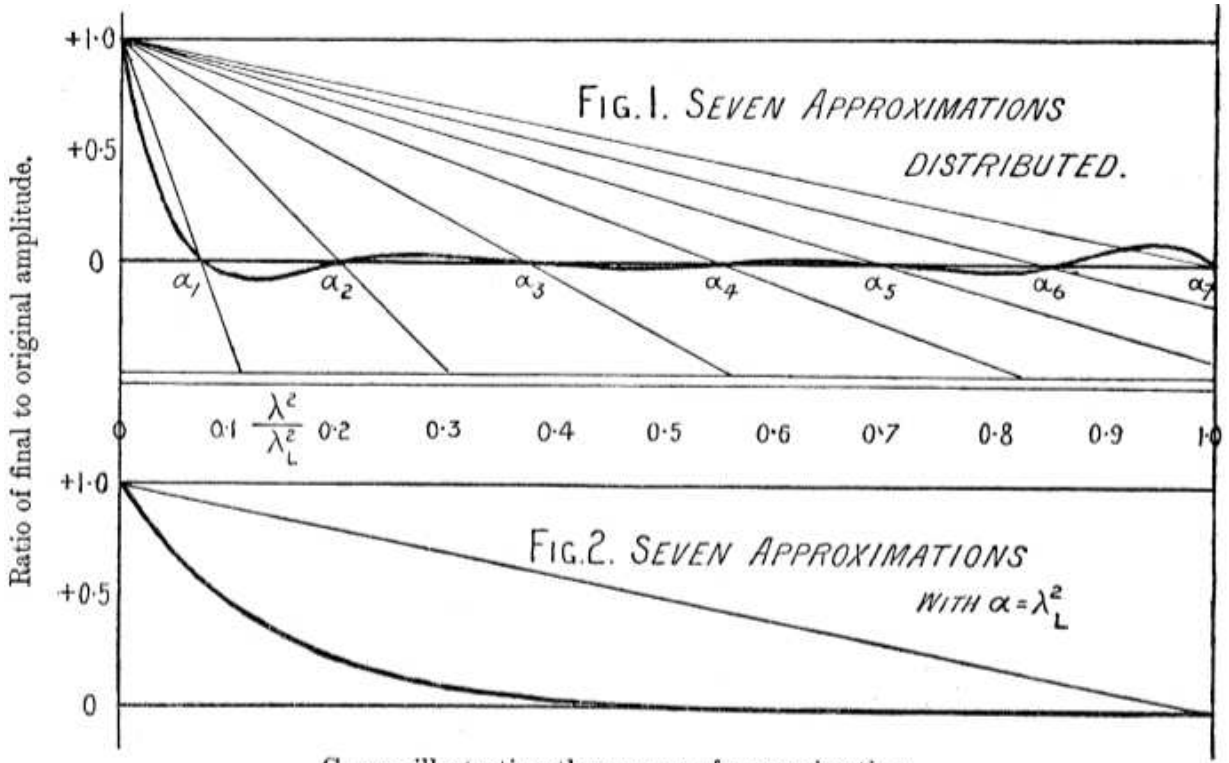
$$\phi_{t+1} - \phi_u = \Sigma \mathrm{A}_k \left(1 - \frac{\lambda_k^2}{\alpha_1}\right)\left(1 - \frac{\lambda_k^2}{\alpha_2}\right) \ldots \left(1 - \frac{\lambda_k^2}{\alpha_t}\right) \mathrm{P}_k \,. \quad . \quad . \quad . \quad . \quad . \quad . \quad (7).$$

A measure of the deviation of two functions from one another which is used in the theory of Least Squares is the sum of the weighted squares of their differences.

Richardson's Minimization

$$\mathrm{SI}\,(\phi_{t+1}-\phi_u)^2 = \Sigma A_k^2 \left[\left(1-\frac{\lambda_k^2}{\alpha_1}\right)\left(1-\frac{\lambda_k^2}{\alpha_2}\right)\times\ldots\times\left(1-\frac{\lambda_k^2}{\alpha_t}\right)\right]^2 \quad . \quad . \quad . \quad (9).$$

Now it has been found that by a judicious choice of $\alpha_1, \alpha_2, \ldots, \alpha_t$, the quantity $\left[\left(1-\frac{\lambda_k^2}{\alpha_1}\right)\left(1-\frac{\lambda_k^2}{\alpha_2}\right)\times\ldots\times\left(1-\frac{\lambda_k^2}{\alpha_t}\right)\right]^2$ may be made small for all possible values of λ_k^2. (Thus fig. 1 shows this done for a set of seven (α)'s. This graph was arrived at by trial.) The error E_{t+1} of ϕ_{t+1} may therefore be made small in comparison with that



Curves illustrating the process of approximation.

Real Richardson's Method

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k(\mathbf{b} - A\mathbf{x}_k) \iff \mathbf{r}_{k+1} = (I - \alpha_k A)\mathbf{r}_k$$

Assume A symmetric and positive definite, and define for $\mu \in \mathbb{R}$ the norm

$$\|\mathbf{r}\|^2_{A^{-\mu}} = \mathbf{r}^T A^{-\mu}\mathbf{r}$$

Using Ritz' idea:

$$Q(\alpha_k) := \|\mathbf{r}_{k+1}\|^2_{A^{-\mu}} \longrightarrow \min .$$

Differentiating with respect to α_k,

$$\frac{dQ}{d\alpha_k} = 2\mathbf{r}^T_{k+1}A^{-\mu}\frac{d\mathbf{r}_{k+1}}{d\alpha_k} = 2((I - \alpha_k A)\mathbf{r}_k)^T A^{-\mu}(-A\mathbf{r}_k) = 0$$

Solving for α_k, we obtain

$$\alpha_k = \frac{\mathbf{r}_k^T A^{1-\mu}\mathbf{r}_k}{\mathbf{r}_k^T A^{2-\mu}\mathbf{r}_k}.$$

Useful choices for μ are 0 and 1

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Conjugate Residuals

For $\mu = 0$, we obtain

$$\alpha_k = \frac{\mathbf{r}_k^T A \mathbf{r}_k}{\|A\mathbf{r}_k\|^2},$$

and we are minimizing in this case locally

$$\|\mathbf{r}_{k+1}\|_2^2 = \|A\mathbf{e}_{k+1}\|_2^2 = \|\mathbf{e}_{k+1}\|_{A^2}^2 \longrightarrow \min.$$

This algorithm has the property

$$\begin{aligned} \mathbf{r}_{k+1}^T A \mathbf{r}_k &= \mathbf{r}_k^T (I - \alpha_k A)^T A \mathbf{r}_k \\ &= \mathbf{r}_k^T A \mathbf{r}_k - \mathbf{r}_k^T \frac{\mathbf{r}_k^T A \mathbf{r}_k}{\|A\mathbf{r}_k\|^2} A^T A \mathbf{r}_k \;=\; 0 \end{aligned}$$

$\Longrightarrow$ **conjugate residuals algorithm**

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Steepest Descent

For $\mu = 1$, we obtain

$$\alpha_k = \frac{\|\mathbf{r}_k\|^2}{\mathbf{r}_k^T A \mathbf{r}_k} \quad \text{and} \quad \|\mathbf{r}_{k+1}\|_{A^{-1}}^2 = \mathbf{r}_{k+1}^T A^{-1} \mathbf{r}_{k+1} \to \min$$

We also minimize $\|\mathbf{e}_{k+1}\|_A^2 = \mathbf{e}_{k+1}^T A \mathbf{e}_{k+1}$, since $A\mathbf{e}_{k+1} = \mathbf{r}_{k+1}$.
We also minimize $Q(\mathbf{x}_k + \alpha \mathbf{r}_k)$ as a function of α, where $Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$, since

$$\frac{dQ}{d\alpha} = \mathbf{r}^T A \mathbf{x} + \alpha \mathbf{r}^T A \mathbf{r} - \mathbf{b}^T \mathbf{r} = 0,$$

leads to the same α.

$$\nabla Q = A\mathbf{x} - \mathbf{b} = -\mathbf{r}$$

$\Longrightarrow$ **method of steepest descent**

Theorem

Steepest descent converges for symmetric positive definite problems.

Best Tactic versus Best Strategy

Choosing α_k such that

$$\|\mathbf{r}_{k+1}\|^2_{A^{-\mu}} \longrightarrow \min$$

is the *best tactic* but maybe not the *best strategy*.
Residual recurrence in Richardson's method:

$$\mathbf{r}_{k+1} = (I - \alpha_k A)\mathbf{r}_k,$$

and since $\mathbf{r}_k = A\mathbf{e}_k$

$$\mathbf{e}_{k+1} = (I - \alpha_k A)\mathbf{e}_k.$$

Thus the error after k steps is

$$\mathbf{e}_k = (I - \alpha_{k-1}A)(I - \alpha_{k-2}A)\cdots(I - \alpha_0 A)\mathbf{e}_0 = P_k(A)\mathbf{e}_0.$$

Definition

The polynomial P_k, which satisfies $P_k(0) = 1$, is called *residual polynomial*.

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Optimal Strategy

Should choose α_k such that the global error is minimized!

Theorem

*If $\alpha_k = \frac{1}{\lambda_k}$, λ_k eigenvalues of A, then convergence is reached in at most n steps (***Proof:** *Cayley-Hamilton)*

Approximation: since

$$\|\mathbf{e}_k\| = \|P_k(A)\mathbf{e}_0\| \leq \|P_k(A)\|\|\mathbf{e}_0\|,$$

can try to minimize $\|P_k(A)\|$. If A is diagonalizable, $A = Q\Lambda Q^{-1}$

$$\|P_k(A)\| = \|QP_k(\Lambda)Q^{-1}\| \leq \|Q\|\|Q^{-1}\|\|P_k(\Lambda)\| = \kappa(Q)\|P_k(\Lambda)\|.$$

For symmetric and positive definite matrices, an interval

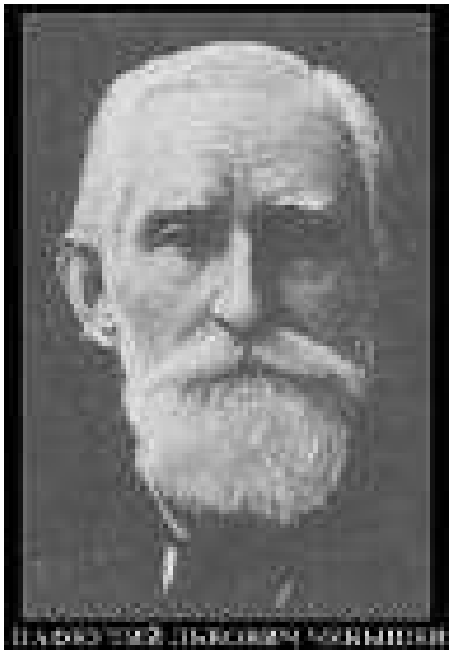
$$0 < a \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq b$$

may be known, and hence

$$\max_i |P_k(\lambda_i)| \leq \max_{a \leq x \leq b} |P_k(x)|.$$

Best Approximation Problems

Chebyshev (1854): Théorie des mécanismes connus sous le nom de parallélogrammes.



Soit $f(x)$ une fonction donnée, U un polynome du degré n avec des coefficients arbitraires. Si l'on choisit ces coefficients de manière à ce que la différence $f(x) - U$, depuis $x = a - h$, jusque à $x = a + h$, reste dans les limites les plus rapprochées de 0, la différence $f(x) - U$ jouira, comme on le sait, de cette propriété:
Parmi les valeurs les plus grandes et les plus petites de la différence $f(x) - U$ entre les limites $x = a - h$, $x = a + h$, on trouve au moins $n+2$ fois la même valeur numérique.

De la Vallée Poussin (1910): Existence, Uniqueness and Equioscillation.

$$\min_{p \in P_n} \max_{x \in K} |f(x) - p(x)|$$

Iterative Methods

Martin J. Gander

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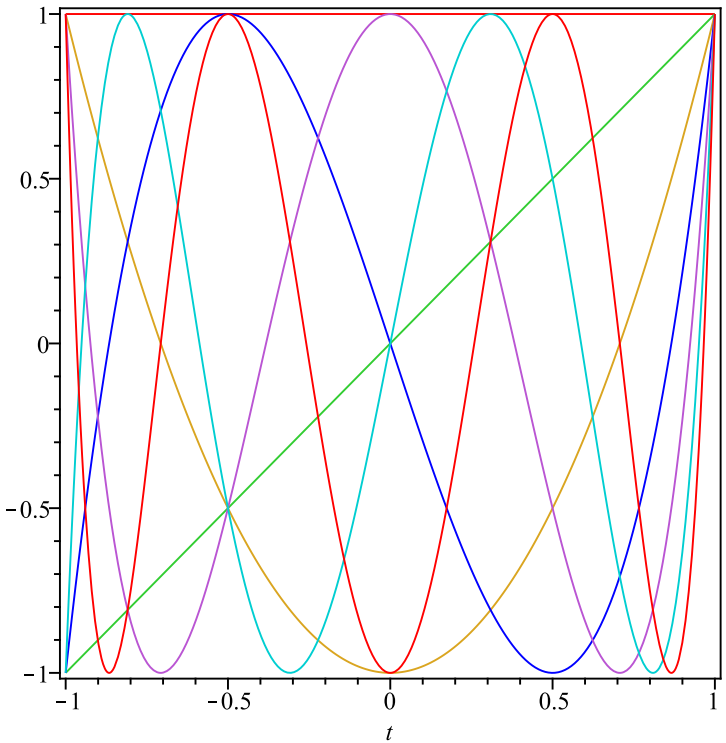
Chebyshev Polynomials

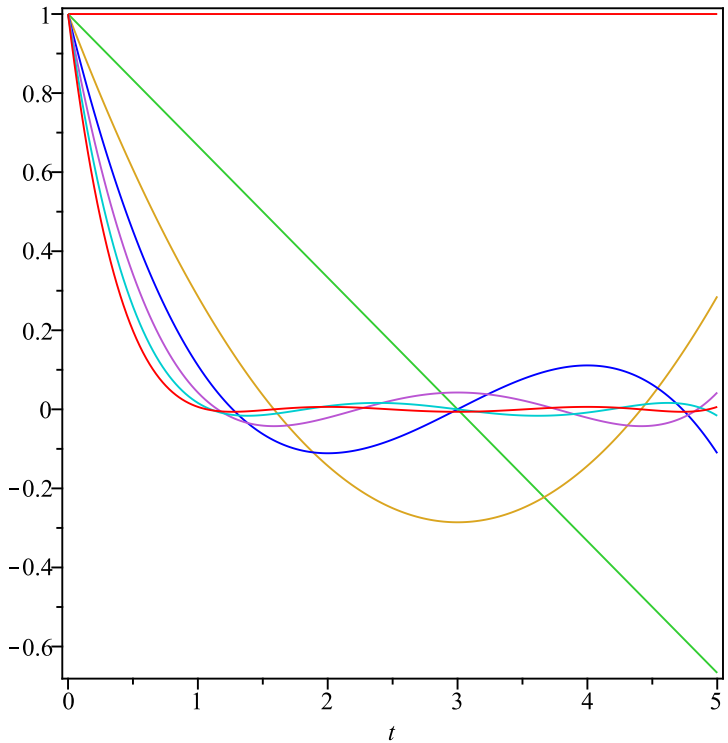
Given a degree k, we want to determine a polynomial P_k with $P_k(0) = 1$ such that

$$\max_{a \le x \le b} |P_k(x)| \longrightarrow \min .$$

Definition (Chebyshev Polynomials)

$$C_k(t) := \cos(k \arccos t), \quad -1 \le t \le 1, \quad k = 0, 1, \ldots$$





Chebyshev Semi-Iterative Method

Normalized Chebyshev polynomial is

$$Q_k(x) = \frac{C_k\left(-1+2\frac{x-a}{b-a}\right)}{C_k\left(\frac{a+b}{a-b}\right)}$$

and can be bounded by

$$\frac{1}{\left|C_k\left(\frac{a+b}{a-b}\right)\right|} \leq 2\left|\frac{\sqrt{\frac{b}{a}}-1}{\sqrt{\frac{b}{a}}+1}\right|^k$$

and we therefore get for this method

$$\|\mathbf{e}_k\| \leq 2\left(\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}\right)^k \|\mathbf{e}_0\|.$$

Richardson's dream comes true in Gene Golub's PhD-thesis (1959): the Chebyshev Semi-Iterative Method!

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Extrapolation Methods

Claude Brezinski (1977): Accélération de la Convergence en Analyse Numérique (Springer)
Avram Sidi and Jacob Bridger (1988): Convergence and stability analyses for some vector extrapolation methods in the presence of defective iteration matrices
Avram Sidi (1991): Efficient implementation of minimal polynomial and reduced rank extrapolation methods

For $A\mathbf{x} = \mathbf{b}$, $A = M - N$, we consider the iteration

$$M\mathbf{x}_{i+1} = N\mathbf{x}_i + \mathbf{b}$$

Idea: find γ_i for $i = 0, 1, \ldots, k$, with $\sum_{i=0}^{k} \gamma_i = 1$ such that

$$\mathbf{y}_k := \sum_{i=0}^{k} \gamma_i \mathbf{x}_i$$

is a much better approximation than $\mathbf{x}_k$.

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Finding a Good Combination

$$\mathbf{x}_i = \mathbf{x} + \mathbf{e}_i \quad \Longrightarrow \quad \underbrace{\sum_{i=0}^{k} \gamma_i \mathbf{x}_i}_{\mathbf{y}_k} = \mathbf{x} \underbrace{\sum_{i=0}^{k} \gamma_i}_{1} + \sum_{i=0}^{k} \gamma_i \mathbf{e}_i,$$

and therefore

$$\mathbf{y}_k = \mathbf{x} + \sum_{i=0}^{k} \gamma_i \mathbf{e}_i.$$

For $\mathbf{y}_k$ to be a good approximation, we would like to have

$$\sum_{i=0}^{k} \gamma_i \mathbf{e}_i \approx 0,$$

and with the error recursion $\mathbf{e}_i = M^{-1}N\mathbf{e}_{i-1} =: G\mathbf{e}_{i-1}$,

$$\sum_{i=0}^{k} \gamma_i G^i \mathbf{e}_0 = P_k(G)\mathbf{e}_0 \approx 0.$$

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An Important Lemma

Lemma

If $P_k(G)\mathbf{e}_0 = 0$, *then for* $m \geq 0$ *also* $P_k(G)\mathbf{e}_m = 0$ *and* $P_k(G)\mathbf{u}_m = 0$, *where* $\mathbf{u}_m := \mathbf{x}_{m+1} - \mathbf{x}_m$.

Proof.

From the recurrence relation, we have

$$\mathbf{u}_m = G\mathbf{u}_{m-1}, \quad \text{and} \quad \mathbf{u}_m = (I - G)\mathbf{e}_m,$$

and since polynomials in G commute, we obtain from $P_k(G)\mathbf{e}_0 = 0$ that

$$0 = G^m P_k(G)\mathbf{e}_0 = P_k(G)G^m\mathbf{e}_0 = P_k(G)\mathbf{e}_m,$$

and similarly

$$0 = (I - G)P_k(G)\mathbf{e}_m = P_k(G)(I - G)\mathbf{e}_m = P_k(G)\mathbf{u}_m.$$

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An Extrapolation Method

Idea: try to approximate $P_k(G)\mathbf{u}_0 \approx 0$. Written with the coefficients of P_k:

$$P_k(G)\mathbf{u}_0 = \gamma_0\mathbf{u}_0 + \gamma_1 \underbrace{G\mathbf{u}_0}_{\mathbf{u}_1} + \cdots + \gamma_k \underbrace{G^k\mathbf{u}_0}_{\mathbf{u}_k} = [\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k]\boldsymbol{\gamma}.$$

Introducing the matrix $U_k \in \mathbb{R}^{n\times(k+1)}$ defined by

$$U_k := [\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k],$$

we would like to determine the coefficients γ_i in the vector $\boldsymbol{\gamma} \in \mathbb{R}^{k+1}$ such that

$$U_k\boldsymbol{\gamma} \approx 0, \quad \text{subject to the constraint} \quad \sum_{i=0}^{k} \gamma_i = 1.$$

Solvable Optimization Problem with Constraint

Removing the Constraint

In order to remove the constraint, we parametrize the γ_i by k parameters ξ_i,

$$\gamma_0 = 1 - \xi_0, \ \gamma_1 = \xi_0 - \xi_1, \ldots, \gamma_i = \xi_{i-1} - \xi_i, \ldots, \gamma_k = \xi_{k-1},$$

which leads to $\boldsymbol{\gamma} = S\boldsymbol{\xi} + \mathbf{e}_1$, $\boldsymbol{\xi} \in \mathbb{R}^k$, with the matrix

$$S = \begin{bmatrix} -1 & & & \\ 1 & -1 & & \\ & 1 & \ddots & \\ & & \ddots & -1 \\ & & & 1 \end{bmatrix}, \quad S \in \mathbb{R}^{(k+1)\times k}.$$

With this new parametrization, we obtain

$$U_k\boldsymbol{\gamma} = U_k S\boldsymbol{\xi} + U_k\mathbf{e}_1 \approx 0.$$

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Extrapolation Methods Continued

The matrix $U_k S$ consists of the columns

$$U_k S = [-\mathbf{u}_0 + \mathbf{u}_1, -\mathbf{u}_1 + \mathbf{u}_2, \ldots, -\mathbf{u}_{k-1} + \mathbf{u}_k].$$

We set $\mathbf{w}_j = \mathbf{u}_{j+1} - \mathbf{u}_j$ and define

$$W_k := [\mathbf{w}_0, \ldots, \mathbf{w}_k] \in \mathbb{R}^{n \times (k+1)}.$$

and thus obtain

$$W_{k-1}\boldsymbol{\xi} \approx -\mathbf{u}_0,$$

$$\mathbf{y}_k = X_k \gamma = X_k S \boldsymbol{\xi} + X_k \mathbf{e}_1 = U_{k-1}\boldsymbol{\xi} + \mathbf{x}_0$$

Solvable optimization problem without constraint

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Krylov Spaces

Definition (Krylov Space)

Let $A \in \mathbb{R}^{n\times n}$ and $\mathbf{r} \in \mathbb{R}^n$. The associated *Krylov space* of dimension k is

$$\mathcal{K}_k(A, \mathbf{r}) = \text{span}\{\mathbf{r}, A\mathbf{r}, A^2\mathbf{r}, \ldots, A^{k-1}\mathbf{r}\}.$$

Since $\mathbf{y}_k = \mathbf{x}_0 + U_{k-1}\boldsymbol{\xi}$, it follows that

$$\mathbf{y}_k - \mathbf{x}_0 = [\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_{k-1}]\boldsymbol{\xi} = [\mathbf{u}_0, G\mathbf{u}_0, \ldots, G^{k-1}\mathbf{u}_0]\boldsymbol{\xi},$$

and therefore this difference lies in a Krylov space,

$$\mathbf{y}_k - \mathbf{x}_0 \in \mathcal{K}_k(G, \mathbf{u}_0).$$

If we choose $\mathbf{x}_0 = 0$, we have $\mathbf{x}_1 = G\mathbf{x}_0 + \mathbf{d} = \mathbf{d}$, and thus $\mathbf{u}_0 = \mathbf{x}_1 - \mathbf{x}_0 = \mathbf{d}$, which implies

$$\mathbf{y}_k \in \mathcal{K}_k(G, \mathbf{d}) = \mathcal{K}_k(M^{-1}N, M^{-1}\mathbf{b}) = \mathcal{K}_k(M^{-1}A, M^{-1}\mathbf{b}).$$

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Minimal Polynomial Extrapolation (MPE)

In order to solve approximately

$$U_k \gamma \approx 0 \quad \text{s.t.} \sum_{j=0}^{k} \gamma_j = 1,$$

MPE fixes the last coefficient to 1 an solves

$$U_{k-1} \mathbf{c} \approx -\mathbf{u}_k$$

using least squares (γ are $\mathbf{c}$ normalized).

Theorem (MPE $\Longleftrightarrow$ FOM)

With γ from MPE, the preconditioned residual

$$\mathbf{r}_k = \mathbf{d} - (I - G)\mathbf{y}_k = M^{-1}(\mathbf{b} - A\mathbf{y}_k)$$

satisfies $\mathbf{r}_k \perp \mathcal{K}_k(G, \mathbf{u}_0)$, and MPE is equivalent to FOM applied to the preconditioned system $M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$.

Topological ε-Algorithm (TEA)

In order to solve approximately

$$U_k \gamma \approx 0 \quad \text{s.t.} \quad \sum_{j=0}^{k} \gamma_j = 1.$$

one can also use a Galerkin approach. Let $Q_{k-1} = [\mathbf{q}, G^T\mathbf{q}, \ldots, (G^T)^{k-1}\mathbf{q}] \in \mathbb{R}^{n\times k}$ and solve

$$Q_{k-1}^T U_k \gamma = 0, \qquad \sum_{j=0}^{k} \gamma_j = 1.$$

Theorem (Equivalence of TEA and NSL)

With $A = M - N$, for any given starting vector $\mathbf{v}_0$, applying non-symmetric Lanczos (NSL) to the preconditioned system $M^{-1}A\mathbf{v} = M^{-1}\mathbf{b}$, or applying TEA to the stationary iterative method $M\mathbf{v}_{k+1} = N\mathbf{v}_k + \mathbf{b}$ with $\mathbf{q} := \mathbf{r}_0 = M^{-1}\mathbf{b} - M^{-1}A\mathbf{v}_0$ leads to identical iterates.

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Preconditioning Arrives Naturally

Every stationary iteration (like multigrid, domain decomposition, etc.) can be written in the form of a stationary iterative method

$$M\mathbf{x}_{k+1} = N\mathbf{x}_k + \mathbf{b} \iff \mathbf{x}_{k+1} = \mathbf{x}_k + M^{-1}(\mathbf{b} - A\mathbf{x}_k)$$

and can therefore serve as a preconditioner for a Krylov method.

For example the restricted additive Schwarz method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \sum_{i=1}^{I} \tilde{R}_i^T A_i^{-1} R_i(\mathbf{b} - A\mathbf{x}_k)$$

The matrix M is called a preconditioner, and the converged solution satisfies the preconditioned system

$$M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$$

Krylov Methods Were not Invented Like This

Stiefel and Rosser 1951: Presentations at a Symposium at the National Bureau of Standards (UCLA)

Hestenes 1951: Iterative methods for solving linear equations

Stiefel 1952: Über einige Methoden der Relaxationsrechnung

Hestenes and Stiefel 1952: Methods of Conjugate Gradients for Solving Linear Systems

"An iterative algorithm is given for solving a system $Ax = k$ of n linear equations in n unknowns. The solution is given in n steps."

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General Idea of Relaxation (following Stiefel)

If A is symmetric and positive definite, we have

$$A\mathbf{u} = \mathbf{f} \quad \Longleftrightarrow \quad F(\mathbf{u}) := \frac{1}{2}\mathbf{u}^T A\mathbf{u} - \mathbf{f}^T\mathbf{u} \longrightarrow \min$$

To solve the minimization problem, a natural relaxation procedure is

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \alpha\mathbf{p}$$

where $\mathbf{p}$ is a search direction and α is the distance to go along this direction.

Example: The Jacobi method

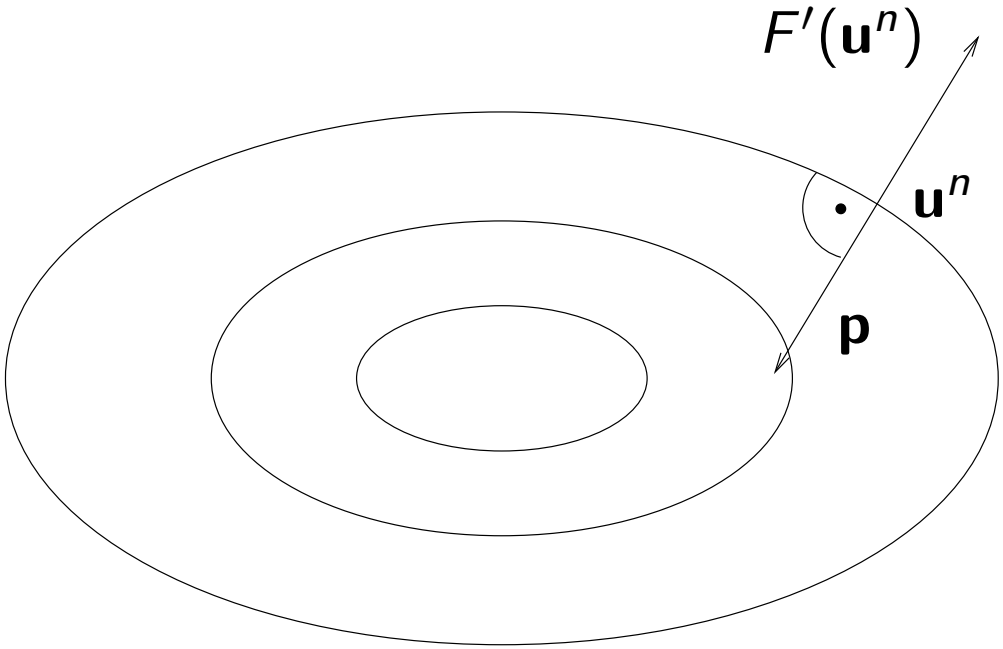
$$\mathbf{u}^{n+1} = \mathbf{u}^n + D^{-1}(\mathbf{f} - A\mathbf{u}^n)$$

for the five point finite difference Laplacian uses

$$\mathbf{p} := (\mathbf{f} - A\mathbf{u}^n) \quad \alpha = \frac{1}{4}.$$

Is the Jacobi Choice a Good One ?

The direction of Jacobi is $\mathbf{p} = (\mathbf{f} - A\mathbf{u}^n) = -F'(\mathbf{u}^n)$, and thus Jacobi goes into the direction of fastest decrease of F at $\mathbf{u}^n$:

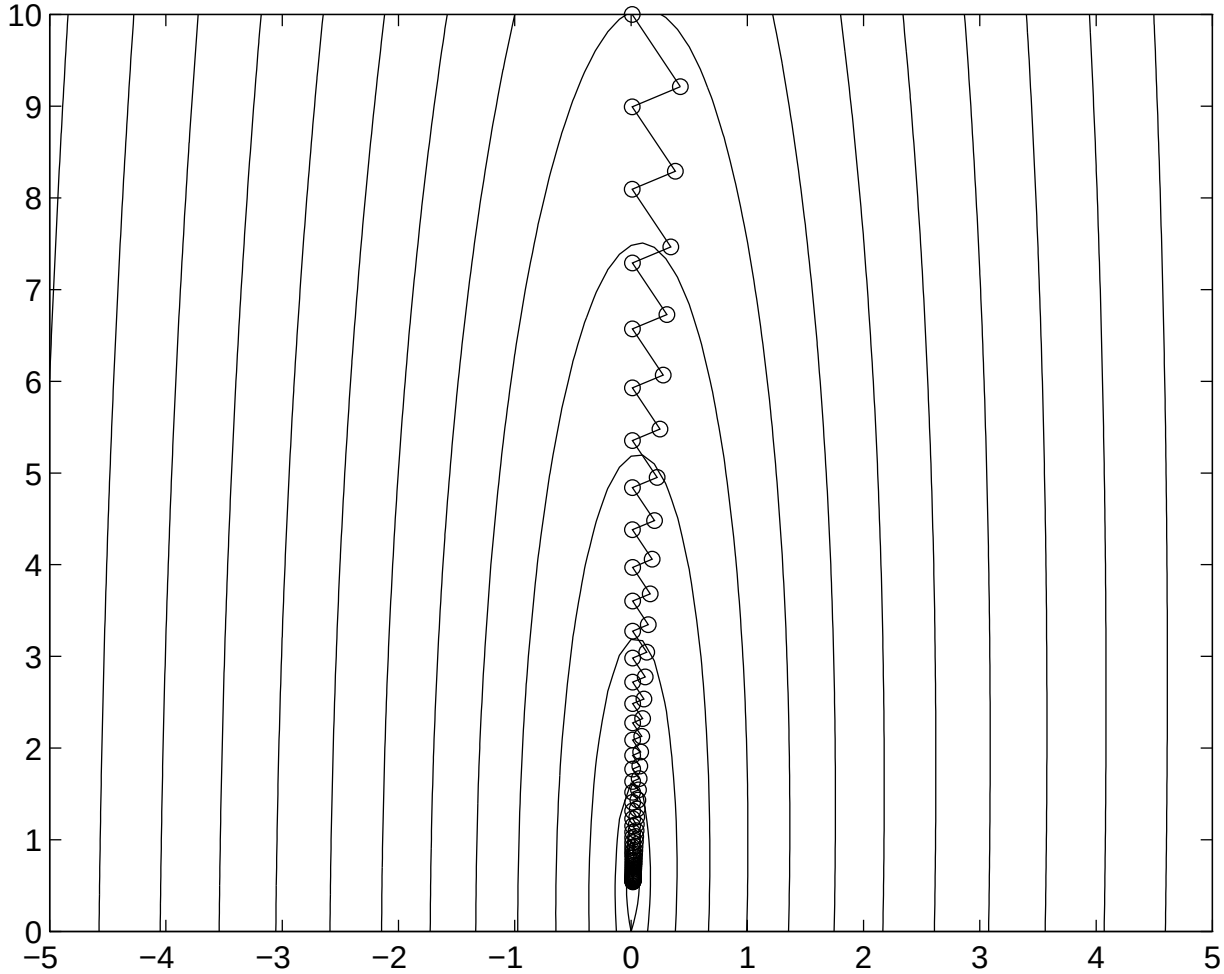


Hence the direction is a good choice, but the distance $\alpha = \frac{1}{4}$ might not be good.

"Ritzscher Gedanke (Stiefel)": Use α to minimize F along the direction $\mathbf{p}$, hence $\alpha = \alpha(n)$:

$$\Longrightarrow \textbf{Method of Steepest Descent}.$$

Problems of Steepest Descent: Cage Syndrome



Stiefel 1952: "Das Auftreten von Käfigen ist eine allgemeine Erscheinung bei Relaxationsverfahren und sehr unerwünscht. Es bewirkt, dass eine Relaxation am Anfang flott vorwärts geht, aber dann immer weniger ausgiebig wird..."

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Remedies Proposed By Stiefel

- Block relaxation: simultaneous relaxation of several equations by the same averaged amount.
- "Scheibenrelaxation":
  1. either choosing search directions related to eigenfunctions on subdomains.
  2. or solving directly small subproblems for low modes by relaxation.

  "Es ist zweckmässig, für einen gegebenen Operator eine Sammlung von Scheiben anzulegen."

  These are precursors of **multigrid methods** and/or **domain decomposition**.
- Conjugate search directions: in that case, one can eliminate completely error components in the direction of each **p**, independent of the other directions.
- "Das n-Schritt Verfahren": the method of **conjugate gradients, (CG)**.

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The Name Krylov Space ?

ИЗВЕСТИЯ АКАДЕМИИ НАУК СССР. 1931

BULLETIN DE L'ACADÉMIE DES SCIENCES DE L'URSS

Classe des sciences mathématiques et naturelles

Отделение математических и естественных наук

Метода Лапласа видимо не удовлетворяла Леверрье, так как в своей статье: «Sur les variations séculaires des éléments des orbites», помещенной в прибавлении к «Connaissance des Temps» за 1843 г., следовательно напечатанной в 1839 или 1840 г., Леверрье излагает свою методу составления векового уравнения. Эта метода включена затем и в его «Recherches Astronomiques» (гл. IX), помещенных в «Annales de l'Observatoire Impérial de Paris» t. II, 1856 г.

Главное неудобство вида (14) векового уравнения для *численного* его решения происходит вследствие того, что члены вида $a_{ii} - \lambda^2$ стоят в диагонали определителя. Это заставило знаменитого математика Якоби поместить в т. XXX журнала «Crelle» составленную им в 1845 г. обширную статью под заглавием: «Ueber ein leichtes Verfahren, die in der Theorie der Secularstörungen vorkommenden Gleichungen numerisch aufzulösen». Эта статья вошла в т. VII собрания сочинений Якоби.

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Topic is Second Order ODEs

Krylov explains a method to solve the system of ODEs

$$\left.\begin{aligned}
\ddot{q}_1 &= a_{11}q_1 + a_{12}q_2 + a_{13}q_3 + \cdots + a_{1k}q_k \\
\ddot{q}_2 &= a_{21}q_1 + a_{22}q_2 + a_{23}q_3 + \cdots + a_{2k}q_k \\
\ddot{q}_3 &= a_{31}q_1 + a_{32}q_2 + a_{33}q_3 + \cdots + a_{3k}q_k \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\ddot{q}_k &= a_{k1}q_1 + a_{k2}q_2 + a_{k3}q_3 + \cdots + a_{kk}q_k
\end{aligned}\right\} \quad \ldots\ldots\ldots(11)$$

Для такой системы при обычном теперь изложении ищут частное решение вида:

$$q_1 = C_1 e^{\lambda t}; \quad q_2 = C_2 e^{\lambda t}; \quad q_3 = C_3 e^{\lambda t} \ldots q_k = C_k e^{\lambda t} \ldots\ldots(12)$$

In order to find the analytical solution, one needs to obtain the eigenvalues λ of the matrix of the system.

Iterative Methods

Martin J. Gander

Storyline

Stationary Methods
- Gauss
- Jacobi
- Seidel
- Modern Notation
- Jacobi
- Gauss-Seidel
- SOR
- Richardson

Non-Stationary
- Richardson
- Conjugate Residuals
- Steepest Descent
- Global Strategies
- Chebyshev
- Semi-Iterative Method
- Extrapolation
- Krylov Spaces
- Preconditioning

Krylov Methods
- Conjugate Gradients
- Stiefel
- Krylov

Conclusions

Computing Eigenvalues

Для совместности этих уравнений необходимо, чтобы было

$$\Delta(\lambda) = \begin{vmatrix} (a_{11} - \lambda^2) & a_{12} & a_{13} & \dots & a_{1k} \\ a_{21} & (a_{22} - \lambda^2) & a_{23} & \dots & a_{2k} \\ a_{31} & a_{32} & (a_{33} - \lambda^2) & \dots & a_{3k} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ a_{k1} & a_{k2} & a_{k3} & \dots & (a_{kk} - \lambda^2) \end{vmatrix} = 0 \dots (14)$$

$$\alpha^k - (a_{11} + a_{22} + a_{33} + \dots + a_{kk})\,\alpha^{k-1}. \quad \dots\dots\dots (21)$$

Отсюда видно, что сумма корней уравнения (19) будет:

$$s_1 = \alpha_1 + \alpha_2 + \dots + \alpha_k = a_{11} + a_{22} + a_{33} + \dots + a_{kk} \quad \dots (22)$$

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Powers of Matrices

Krylov now explains the method of Leverrier

$$\left.\begin{aligned} q_1^{IV} &= a_{11}\ddot{q}_1 + a_{12}\ddot{q}_2 + \cdots + a_{1k}\ddot{q}_k \\ q_2^{IV} &= a_{12}\ddot{q}_1 + a_{22}\ddot{q}_2 + \cdots + a_{2k}\ddot{q}_k \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ q_k^{IV} &= a_{k1}\ddot{q}_1 + a_{k2}\ddot{q}_2 + \cdots + a_{2k}\ddot{q}_k \end{aligned}\right\} \quad \ldots\ldots\ldots(23)$$

$$\left.\begin{aligned} q_1^{IV} &= b_{11}q_1 + b_{12}q_2 + b_{13}q_3 + \cdots + b_{1k}q_k \\ q_2^{IV} &= b_{21}q_1 + b_{22}q_2 + b_{23}q_3 + \cdots + b_{2k}q_k \\ q_3^{IV} &= b_{31}q_1 + b_{32}q_2 + b_{33}q_3 + \cdots + b_{3k}q_k \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ q_k^{IV} &= b_{k1}q_1 + b_{k2}q_2 + b_{k3}q_3 + \cdots + b_{kk}q_k \end{aligned}\right\} \quad \ldots\ldots\ldots(26)$$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1k} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2k} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3k} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{k1} & a_{k2} & a_{k3} & \cdots & a_{kk} \end{vmatrix} \cdot \begin{vmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1k} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2k} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3k} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{k1} & a_{k2} & a_{k3} & \cdots & a_{kk} \end{vmatrix} = \begin{vmatrix} b_{11} & b_{12} & b_{13} & \cdots & b_{1k} \\ b_{21} & b_{22} & b_{23} & \cdots & b_{2k} \\ b_{31} & b_{32} & b_{33} & \cdots & b_{3k} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ b_{k1} & b_{k2} & b_{k3} & \cdots & b_{kk} \end{vmatrix} \quad (27)$$

Powers of Matrices

$$s_2 = \alpha_1^2 + \alpha_2^2 + \alpha_3^2 + \cdots + \alpha_k^2 = b_{11} + b_{22} + b_{33} + \cdots + b_{kk} \quad \ldots(30)$$

$$\begin{vmatrix} b_{11} & b_{12} & \ldots & b_{1k} \\ b_{21} & b_{22} & \ldots & b_{2k} \\ \ldots & \ldots & \ldots & \ldots \\ b_{k1} & b_{k2} & \ldots & b_{kk} \end{vmatrix} \cdot \begin{vmatrix} a_{11} & a_{12} & \ldots & a_{1k} \\ a_{21} & a_{22} & \ldots & a_{2k} \\ \ldots & \ldots & \ldots & \ldots \\ a_{k1} & a_{k2} & \ldots & a_{kk} \end{vmatrix} = \begin{vmatrix} c_{11} & c_{12} & \ldots & c_{1k} \\ c_{21} & c_{22} & \ldots & c_{2k} \\ \ldots & \ldots & \ldots & \ldots \\ c_{k1} & c_{k2} & \ldots & c_{kk} \end{vmatrix} \quad \ldots\ldots(32)$$

$$s_3 = \alpha_1^3 + \alpha_2^3 + \alpha_3^3 + \cdots + \alpha_k^3 = c_{11} + c_{22} + c_{33} + \cdots + c_{kk}. \quad \ldots(33)$$

Продолжая поступать таким образом получим последовательно значения

$$\left.\begin{aligned} s_4 &= \alpha_1^4 + \alpha_2^4 + \alpha_3^4 + \cdots + \alpha_k^4 \\ s_5 &= \alpha_1^5 + \alpha_2^5 + \alpha_3^5 + \cdots + \alpha_k^5 \\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ s_k &= \alpha_1^k + \alpha_2^k + \alpha_3^k + \cdots + \alpha_k^k \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots(34)$$

Using Newton's Formulas

Krylov arrives at the general characteristic polynomial

$$\Delta(\alpha) = \alpha^k + B_1 \alpha^{k-1} + B_2 \alpha^{k-2} + \cdots + B_k = 0. \quad \ldots\ldots (35)$$

using the s_i and the well known Newton formulas

Зная значения

$$s_1,\ s_2,\ s_3 \ldots s_k$$

найдем коэфициенты $B_1, B_2 \ldots B_k$ по известным формулам Ньютона:

$$\left.\begin{aligned}
0 &= s_1 + B_1 \\
0 &= s_2 + B_1 s_1 + 2B_2 \\
0 &= s_3 + B_1 s_2 + B_2 s_1 + 3B_3 \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 &= s_{k-1} + B_1 s_{k-2} + B_2 s_{k-3} + \cdots + B_{k-2} s_1 + (k-1) B_{k-1} \\
0 &= s_k + B_1 s_{k-1} + B_2 s_{k-2} + \cdots + B_{k-1} s_1 + k B_k
\end{aligned}\right\} \ldots (36)$$

Is this really the origin of Krylov spaces ?

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Conclusions

Conclusions

- **Stationary iterative methods:**
  - Jacobi
  - Gauss-Seidel
  - SOR
- **Non-Stationary iterative methods:**
  - Richardson
  - Chebyshev Semi-iterative method
  - Conjugate Gradients
  - Krylov methods in general (MINRES, SYMLQ, GMRES, FOM, QMR, BiCGStab, ...)
- **Preconditioning:**
  - Comes very naturally from stationary iterative methods (Diagonal (Jacobi), Multigrid, Domain Decomposition, ...)
  - Always use a Krylov accelerator

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