Lecture W5

Remark:

If one deals with complex system (System with complex coeffs.), i.e., $A\vec{x}=\vec{b}$, a_{ik}, x_i or b_i are complex numbers, then (i) all methods can be used with complex arithmetics instead of real arithmetics or (ii) the real system of twice the original size can be solved:

$$(A+iC)(\vec{x}+i\vec{y}) = (\vec{b}+i\vec{d})$$

$$A\vec{x} + iC\vec{x} + iA\vec{y} - C\vec{y} = \vec{b} + i\vec{d} \Longrightarrow$$

$$\begin{cases} A\vec{x} - C\vec{y} = \vec{b} \\ C\vec{x} + A\vec{y} = \vec{d} \end{cases} \Longleftrightarrow \begin{pmatrix} A & -C \\ C & A \end{pmatrix} \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ \vec{d} \end{pmatrix}$$

Block matrix of $2N \times 2N$ size.

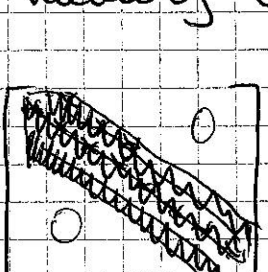
Sparse Linear Systems

DF: A system of eqs is called sparse if only a relatively small number of its matrix elements a_{ij} are nonzero.

!! One can reduce memory usage and/or time (n. of steps)

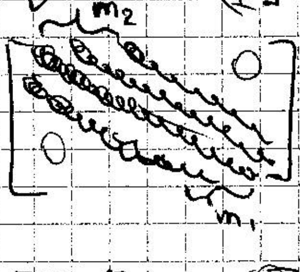
Examples:

1) tridiagonal matrices



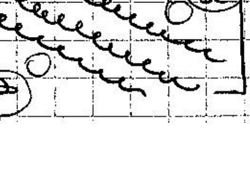
only diagonal ± one column have nonzero elements.

2) Band matrices



only elements along a few diagonal lines adjacent to the main diagonal are nonzero.

3) Cyclic tridiagonal → finite diff. with PBC.



→ tridiagonal with nonzero corners.

Tridiagonal

$$A = \begin{pmatrix} b_1 & c_1 & 0 & \dots & 0 \\ a_2 & b_2 & c_2 & & \\ & a_3 & b_3 & c_3 & \\ 0 & & \ddots & \ddots & c_{n-1} \\ & & & a_n & b_n \end{pmatrix} = \underbrace{\begin{pmatrix} \boxed{\beta_1} & 0 & & \\ \alpha_2 & \beta_2 & & \\ & \alpha_3 & \beta_3 & \\ 0 & & \alpha_n & \beta_n \end{pmatrix}}_{\text{III } L} \underbrace{\begin{pmatrix} 1 & \boxed{\gamma_1} & & \\ & 1 & \gamma_2 & \\ & & 1 & \gamma_3 \\ 0 & & & \ddots\ 1 \end{pmatrix}}_{\text{III } U}$$

- $A = LU$ - exist if A is strongly non singular.
- one makes LU-decomposition without pivoting.

I)

$$\begin{cases} b_1 = \beta_1 \\ a_i = \alpha_i & i = 2, n \\ b_i = \alpha_i \gamma_{i-1} + \beta_i & ; i = 2, n \\ c_i = \beta_i \gamma_i & ; i = 1, n-1 \end{cases} \Rightarrow \boxed{\begin{cases} \gamma_i = c_i / \beta_i & \\ \beta_{i+1} = b_{i+1} - \alpha_{i+1} \gamma_i & ; i = 1, n-1 \end{cases} \text{ with } \underline{\beta_1 = b_1} \text{ and } \underline{\alpha_i = a_i}}$$

forward → LU decomp.

$(n-1)$ multiplications and divisions

II $\quad LU\vec{x} = \vec{f} \Rightarrow U\vec{x} = \vec{g} \Rightarrow L\vec{g} = \vec{f} \Rightarrow$ $O(n)$

$$\begin{pmatrix} \beta_1 & 0 & & \\ \alpha_2 & \beta_2 & & \\ & \alpha_3 & \beta_3 & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix} \Rightarrow$$

$$\begin{cases} g_1 = \dfrac{f_1}{\beta_1} \\ g_{i-1}\alpha_i + g_i \beta_i = f_i \end{cases} \Rightarrow \begin{cases} g_1 = \dfrac{f_1}{\beta_1} \\ g_i = \dfrac{f_i - g_{i-1}\alpha_i}{\beta_i} & i = 2, n \end{cases} \to O(n)$$

$$\begin{pmatrix} 1 & \gamma_1 & & \\ & 1 & \gamma_2 & \\ & & 1 & \gamma_3 \\ & & & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} g_1 \\ \vdots \\ g_n \end{pmatrix} \Rightarrow \begin{cases} x_n = g_n \\ x_i = g_i - \gamma_i x_{i+1} \\ i = n-1, \dots 1 \end{cases}$$

① LU - for tridiagonal matrices is $O(n)$ in contrast with LU for non-sparse matrix ($O(n^3)$)

② Allows memory saving by storing only non-zero elements and their positions.

"Almost band matrices"

What happens with inverse of A, if we change one or few elements in A?

$$\vec{u} \otimes \vec{v} \equiv \begin{pmatrix} u_1 v_1 & u_1 v_2 & \dots \\ u_2 v_2 & u_2 v_2 & \dots \\ \dots & & \end{pmatrix} \Rightarrow$$

$$A + \vec{e}_i \otimes \vec{e}_j \cdot a \to \text{adds } a \text{ to } a_{ij}$$

$$(A + \vec{u} \otimes \vec{v})^{-1} = \left(A\left(\mathbb{1} + A^{-1}\underline{u}\otimes\underline{v}\right)\right)^{-1} = \underbrace{\left(\mathbb{1} + A^{-1}\underline{u}\otimes\underline{v}\right)^{-1}} A^{-1} =$$

$$= \left\{ \frac{1}{1+\lambda} = 1 - \lambda + \lambda^2 - \dots \right\} = \text{formal series extension}$$

$$= \left(\mathbb{1} - A^{-1}\underline{u}\otimes\underline{v} + A^{-1}\underline{u}\otimes\underline{v}\, A^{-1}\underline{u}\otimes\underline{v} - \dots\right) A^{-1} =$$

$$= A^{-1} - \underbrace{A^{-1}u\otimes\underline{v}A^{-1}} + \underbrace{A^{-1}\underline{u}\otimes\underline{v}A^{-1}}\underline{u}\otimes\underline{v}A^{-1} - \dots =$$

$$= A^{-1} - A^{-1}\underline{u}\otimes\underline{v}A^{-1}\Big(1 - \underbrace{\underline{u}\otimes\underline{v}\cdot A^{-1}}_{\lambda} + \underbrace{\underline{u}\otimes\underline{v}A^{-1}\underline{u}\otimes\underline{v}A^{-1}}_{\lambda^2} + \Big) = \frac{1}{1+\lambda}$$

$$= \boxed{A^{-1} - \frac{(A^{-1}\underline{u})\cdot(\underline{v}A^{-1})}{1 + u\cdot(vA^{-1})} = (A + \underline{u}\otimes\underline{v})^{-1}}$$

1) $\vec{z} = A^{-1}\vec{u}$; $\vec{w} = \vec{v}A^{-1}$; $\lambda = \vec{u}\cdot\vec{w} \Rightarrow A^{-1} - \dfrac{\vec{z}\otimes\vec{w}}{1+\lambda}$

$\downarrow O(N^2)$ $\quad\downarrow O(N^2)$ $\quad\downarrow O(N^2)$ $\quad\downarrow O(N^2)$

Then: for $(A + \underline{u} \otimes \underline{v})\vec{x} = \vec{b}$ (Or alternatively two problems.)

if $A\vec{y} = \vec{b}$ and $A\vec{z} = \vec{u}$ $\Rightarrow$

$$\vec{x} = (A + \underline{u} \otimes \underline{v})^{-1}\vec{b} = \underbrace{A^{-1}\vec{b}}_{=\vec{y}} + \frac{\overbrace{(A^{-1}u)}^{\vec{z}}\overbrace{(vA^{-1})b}^{\vec{y}}}{1 + u(vA^{-1})}$$

$$v(A^{-1}u) = \underline{v}\cdot\underline{z}$$

$$\boxed{\underline{x} = \vec{y} - \left(\frac{\vec{z}\cdot\vec{v}}{1 + \vec{v}\cdot\vec{z}}\right)\vec{y}}$$

Cyclic tridiagonal. → finite diff.

tridiagonal A

$$\begin{pmatrix} b_1 & c_1 & & 0 & \beta \\ a_2 & b_2 & c_2 & & \\ 0 & a_3 & \ddots & & \\ & 0 & & \ddots & \\ \alpha & & & 0 & b_n \end{pmatrix} = \begin{pmatrix} b_1' & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & a_3 & b_3 & c_3 & \\ & & \ddots & \ddots & c_{n-1} \\ & & & a_n & b_n' \end{pmatrix} +$$

$$+ \begin{pmatrix} \gamma \\ 0 \\ \vdots \\ 0 \\ \alpha \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \beta/\gamma \end{pmatrix}, \quad \text{here } \underline{u} \otimes \underline{v} = \begin{pmatrix} \gamma & & \beta \\ & 0 & \\ \alpha & & \frac{\alpha\beta}{\gamma} \end{pmatrix}$$

$$\underline{u} \qquad \underline{v}$$

$$\begin{cases} b_1 = b_1' + \gamma \\ b_N = b_n' + \frac{\alpha\beta}{\gamma} \end{cases} \Rightarrow \underline{\underline{\begin{cases} b_1' = b_1 - \gamma \\ b_N' = b_N - \frac{\alpha\beta}{\gamma} \end{cases}}}, \quad \gamma = -b_1$$

$$A\underset{\approx}{\vec{y}} = \vec{b}, \quad A\vec{z} = \underset{\approx}{\vec{u}}$$

□

Special non-sparse matrices.

1) Toeplitz - matrix having constants along diagonals

$$\begin{bmatrix} a_0 & a_1 & a_2 & \cdots \\ a_{-1} & a_0 & a_1 & \cdots \\ a_{-2} & a_{-1} & a_0 & \cdots \\ & & & \ddots \end{bmatrix}$$

$(2n-1)$ elements $\left[n^2 \text{ in normal case} \right]$

- signal processing; diff. and integral eqs, etc.

2) Symmetric positive definite matrices

$$a_{ij} = a_{ji} \text{ or } A = A^T \qquad \vec{v}\cdot A\cdot\vec{v} > 0 \quad \forall \vec{v}$$

Cholesky decomposition $A = LL^T$, L lower triangular.

$$\begin{pmatrix} l_{11} & & & \\ l_{21} & l_{22} & & 0 \\ l_{31} & l_{32} & l_{33} & \\ \dots & \dots & \dots & l_{nn} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31} & \\ & l_{22} & l_{32} & \\ & & l_{33} & \\ 0 & & & \ddots \; l_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & a_{31} & \dots \\ \boxed{a_{21}} & a_{22} & a_{32} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \dots & \dots & \dots & \end{pmatrix}$$

$$\begin{cases} a_{11} = l_{11}^2 \\ a_{22} = l_{21} l_{21}^2 + l_{22}^2 \\ a_{33} = l_{31}^2 + l_{32}^2 + l_{33}^2 \end{cases} \Rightarrow a_{ii} = \sum_{k=1}^{i-1} l_{ki}^2 + l_{ii}^2$$

$i = 1, n$

$$l_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} l_{ki}^2} \qquad (1)$$

$$\begin{cases} a_{21} = l_{21} a_{11} + l_{22} a_{21} \\ a_{31} = l_{31} l_{11} + l_{32} l_{21} + l_{33} l_{31} \qquad a_{\underset{ij}{32}} = l_{31} l_{21} + l_{32} l_{22} + l_{33} l_{\underset{ij}{32}} \\ \cancel{a_{ij} = l_{ij} a_{jj} + l_{i2} a_{21}} \end{cases}$$

$$a_{ij} = l_{i1} l_{j1} + l_{i2} l_{j2} + l_{i3} l_{j3} + \dots \; l_{ii} l_{ij}$$

$$a_{ij} = \sum_{k=1}^{i-1} l_{ik} a_{jk} + l_{ii} l_{ij}$$

$$\Downarrow$$

$$\boxed{l_{ij} = \frac{1}{l_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} L_{ik} L_{jk} \right) \quad j = i+1, N} \qquad (2)$$

(3) Standard LU backsubstitution.

$O\left(\frac{n^3}{6}\right)$ in contrast with Gauss/LU $O\left(\frac{n^3}{3}\right)$

two times faster.

Iterative Improvement

1) $A\vec{x} = \vec{b}$ $\qquad \vec{x}_{old} = \vec{x} + \delta\vec{x}$ – numerical approx.

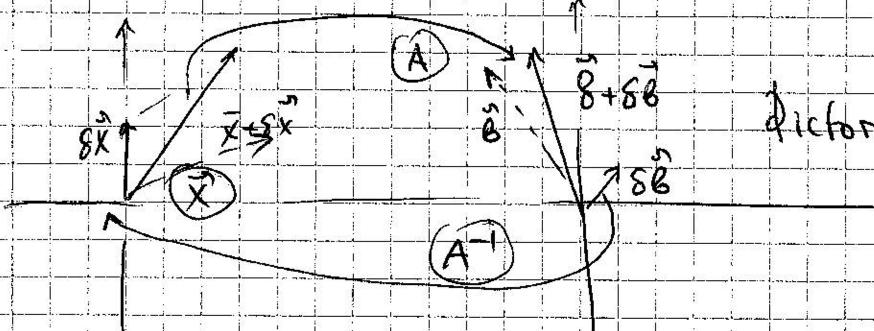
$\vec{x}$: exact solution

$$A(\vec{x}+\delta\vec{x}) = (\vec{b}+\delta\vec{b})$$

$$A\cdot\delta\vec{x} = \delta\vec{b} \quad (*)$$ but LU is known $\Rightarrow$ (*) can be solved for $\delta\vec{x}$ & for $\delta\vec{b}$.

$$A\cdot\delta\vec{x} = \left(A(\vec{x}+\delta\vec{x}) - \vec{b}\right) \Rightarrow \vec{x}_{new} = \vec{x}_{old} - \delta\vec{x}$$

Pictorial illustration



2) But LU decomposition is also obtained with approximation, i.e., $A^{-1} \approx B_0 \Rightarrow B_0 A \approx \mathbb{1}$

$R \equiv 1 - B_0\cdot A$ – residual Matrix.

$B_0 A = 1 - R$

$$A^{-1} = A^{-1}(B_0^{-1}B_0) = (A^{-1}B_0^{-1})B_0 = (B_0A)^{-1}B_0 =$$

$$= (1-R)^{-1}B_0 = \left\{\begin{array}{l}\text{formal}\\ \text{expansion}\end{array}\right\} = (1+R+R^2+\dots)B_0$$

Let $B_n \equiv (1+R+\dots R^n)B_0$; $B_n \xrightarrow[n\to\infty]{} A^{-1}$

and $\vec{x}_n = B_n\vec{b}$ n-th approximation.

$$\underline{x}_{n+1} = B_{n+1}\underline{b} = (1+R+\dots R^{n+1})B_0\underline{b} =$$

$$= (B_0 + RB_0 + \dots R^{n+1}B_0)\underline{b} =$$

$$= [B_0 + R(B_0 + \dots R^nB_0)]\underline{b} =$$

$$= B_0\underline{b} + R(1+\cdots R^n)B_0\underline{b} = B_0\underline{b} + RB_n\underline{b} =$$
$$= (B_0 + RB_n)\underline{b} = (B_0 + B_n - B_n + RB_n)\underline{b} =$$
$$= (B_0 + B_n - (1-R)B_n)\underline{b} = \{(1-R) \equiv B_0 A\} =$$
$$= (B_n + B_0 - B_0 A B_n)\underline{b} = \underbrace{B_n\underline{b}}_{\underline{x}_n} + B_0(1 - AB_n)\underline{b} =$$

$$= \boxed{\underline{x}_n + B_0(\underline{b} - A\underline{x}_n) = \underline{x}_{n+1}}$$

$$\delta\underline{x} \equiv -(\underline{x}_{n+1} - \underline{x}_n) = -B_0(\underline{b} - A\underline{x}_n) = \{B_0 \approx A^{-1}\} = B_0(A\underline{x}_n - \underline{b})$$

$$\delta\underline{x} = A^{-1}\big(\underbrace{A(\underline{x}+\delta\underline{x})}_{\underline{x}_n} - \underline{b}\big)$$

!! In iterative improvement one do not need exact A^{-1} (or LU decomposition), one only need small R.

System Conditioning

DF: if the small changes in initial data cause big changes in the solution, then the problem is called ill-conditioned.

$$A\underline{x} = \underline{b}\ ; \to A(\underline{x} + \delta\underline{x}_1) = \underline{b} + \Delta\underline{b}$$
$$\to (A + \Delta A)(\underline{x} + \delta\underline{x}_2) = \underline{b}$$
$$\to (A + \Delta A)(\underline{x} + \delta\underline{x}_3) = \underline{b} + \Delta\underline{b}$$

! How the elements of A^{-1} will change if elements of A are changed?

$$A A^{-1} = E$$

$$\frac{\partial(A A^{-1})}{\partial a_{ij}} = \frac{\partial A}{\partial a_{ij}} A^{-1} + A\frac{\partial A^{-1}}{\partial a_{ij}} = 0 \Rightarrow \frac{\partial(A^{-1})}{\partial a_{ij}} = -A^{-1}\frac{\partial A}{\partial a_{ij}} A^{-1}$$

$$\frac{\partial A}{\partial a_{ij}} = e_{ij}\ ;$$ $\to$ matrix with nonzero element at i,j.

$$\frac{\partial A^{-1}}{\partial a_{ij}} = -A^{-1} e_{ij} A^{-1} \Rightarrow \{\text{for examp.}\} = -A^{-1} e_{i1} e_{1j} A^{-1} =$$

$$= -\begin{bmatrix} \alpha_{1i} & \\ \alpha_{2i} & O \\ \vdots & \\ \alpha_{ni} & \end{bmatrix} \begin{bmatrix} \alpha_{j1} & \alpha_{j2} & \dots & \alpha_{jn} \\ & O & & \end{bmatrix} =$$

$$\left[\frac{\partial A^{-1}}{\partial a_{ij}}\right]_{kl} = -\begin{bmatrix} \alpha_{1i}\alpha_{j1} & \alpha_{1i}\alpha_{j2} & \dots & \alpha_{1i}\alpha_{jn} \\ & & & \\ \alpha_{ni}\alpha_{j1} & & \dots & \alpha_{ni}\alpha_{jn} \end{bmatrix} \rightarrow$$

$$\frac{\partial \alpha_{kl}}{\partial a_{ij}} = -\alpha_{ki}\alpha_{jl} \Rightarrow \boxed{d\alpha_{kl} = -\alpha_{ki}\alpha_{jl}\, da_{ij}}$$

if da_{ij} is small, but α_{ki} and/or α_{jl} are large
$\Rightarrow d\alpha_{kl}$ is large.

1) small determinant $\rightarrow$ large elements of inverse matrix $\rightarrow$ ill-conditioning $\Rightarrow$ system is also ill-conditioned.

$$A\underline{x} = \underline{b} \Rightarrow \underline{x} = A^{-1}\underline{b}$$

1) $$\frac{\partial \underline{x}}{\partial a_{ij}} = \frac{\partial A^{-1}}{\partial a_{ij}} \vec{b} = -A^{-1} e_{ij} A^{-1} \vec{b} = -A^{-1} e_{ij} \vec{x} =$$

$$= -\begin{pmatrix} \alpha_{1i} & \\ \alpha_{2i} & O \\ \vdots & \\ \alpha_{ni} & \end{pmatrix} \vec{x} = -\begin{pmatrix} \alpha_{1i} x_1 \\ \vdots \\ \alpha_{ni} x_n \end{pmatrix} \Rightarrow$$

$$\left(\frac{\partial \underline{x}}{\partial a_{ij}}\right)_k = -\alpha_{ki} x_j \Rightarrow \boxed{dx_k = -\alpha_{ki} x_j\, da_{ij}}$$

large $dx_k \rightarrow$ large.

2) $$\frac{\partial \underline{x}}{\partial b_i} = A^{-1} \frac{\partial \underline{b}}{\partial b_i} = A^{-1} \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \end{pmatrix} i = \begin{pmatrix} \alpha_{1i} \\ \vdots \\ \alpha_{ii} \\ \vdots \\ \alpha_{ni} \end{pmatrix} \Rightarrow$$

$$\Rightarrow \left(\frac{\partial x}{\partial b_i}\right)_k = \alpha_{ki} \Rightarrow \boxed{dx_k = \alpha_{ki}\, db_i}$$

Conclusion: if elements of inverse matrix are large $\Rightarrow$ small variations in matrix elements and/or free terms lead to large variation in solution.

- Absolute error for variation in $\vec{b}$

$$dx_k = \alpha_{ki} b_i \Rightarrow \text{due to } db_i \text{ element } i$$

$$dx_k = \sum_i \alpha_{ki} db_i \Rightarrow \text{due to all elements} \Rightarrow$$

matrix form $\boxed{d\vec{x} = A^{-1} d\vec{b}}$ $\Leftarrow$ $A(\underline{x}+d\underline{x}) = \underline{b} + db$, $Ax = b \Rightarrow Ad\underline{x} = db$

$$\|d\vec{x}\| = \|A^{-1} d\vec{b}\| \le \underline{\underline{\|A^{-1}\|}} \|d\vec{b}\|, \text{ where}$$

$$\|\vec{x}\| = \sqrt{\sum_i x_i^2}; \quad \|A\| = \sqrt{\sum_i \sum_k a_{ik}^2}$$

- Relative error for $(d\vec{b})$

$$\vec{b} = A\vec{x} \Rightarrow \|\vec{b}\| \le \|A\| \|\vec{x}\|$$

$$\frac{1}{\|x\|} \le \frac{\|A\|}{\|b\|} \qquad \|dx\| \le \|A^{-1}\| \|d\vec{b}\|$$

$$\Downarrow$$

$$\frac{\|dx\|}{\|x\|} \le \|A\| \|A^{-1}\| \frac{\|d\vec{b}\|}{\|b\|}; \quad \|A\| \|A^{-1}\| \equiv \text{cond}(A)$$

- Relative error for (dA)

$$dx_k = \sum_{ij} \alpha_{kj} x_j da_{ij} \Rightarrow d\vec{x} = -A_0^{-1} \vec{x} \, dA$$

$$d\vec{x} = -(A+dA)^{-1} dA \, \vec{x}$$

$$\|d\vec{x}\| \le \|(A+dA)^{-1}\| \|dA\| \|x\|$$

$$\frac{\|d\vec{x}\|}{\|x\|} \le \|(A+dA)^{-1}\| \|dA\|$$

$$\boxed{\text{if } \|A\| < 1 \Rightarrow \|(1+A)^{-1}\| \le \frac{1}{1-\|A\|}}$$

$$\|(A+dA)^{-1}\| = \|(1 + A^{-1}dA)^{-1} A^{-1}\| = \{\text{if } \|A^{-1}dA\| < 1\} \Rightarrow$$

$$\le \frac{1}{1-\|A^{-1}dA\|} \|A^{-1}\|$$

$$\frac{\|d\vec{x}\|}{\|x\|} \leq \frac{1}{1-\|A^{-1}dA\|}\|A^{-1}\|\|dA\|$$

$$\leq \frac{\|A^{-1}\|\|dA\|}{\left(1-\|A^{-1}\|\|dA\|\cdot\frac{\|A\|}{\|A\|}\right)}\frac{\|A\|}{\|A\|}$$

$$= \frac{\|A^{-1}\|\|A\|}{1-\|A^{-1}\|\|A\|\frac{\|dA\|}{\|A\|}}\frac{\|dA\|}{\|A\|} \Rightarrow$$

$$\frac{\|d\vec{x}\|}{\|x\|} \leq \frac{\mathrm{cond}(A)}{1-\mathrm{cond}(A)\frac{\|dA\|}{\|A\|}}\cdot\frac{\|dA\|}{\|A\|} \quad ; \text{ if } \|A^{-1}dA\| < 1$$