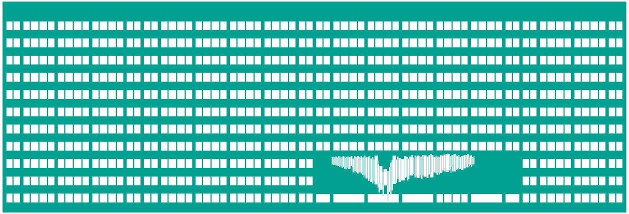
VŠB TECHNICKÁ UNIVERZITA OSTRAVA

VSB TECHNICAL UNIVERSITY OF OSTRAVA



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Numerická lineární algebra 1

QR rozklad

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VŠB TECHNICKÁ UNIVERZITA OSTRAVA | IT4INNOVATIONS NÁRODNÍ SUPERPOČÍTAČOVÉ CENTRUM

QR rozklad

Definice

Čtvercová matice Q, která splňuje $Q^T Q = I$ se nazývá ortogonální matice. Ortogonální matice má ortonormální sloupce a splňuje $Q^{-1} = Q^T$.

- Pro sloupce Q platí

$$(\boldsymbol{q}_i, \boldsymbol{q}_j) = \boldsymbol{q}_i^T \boldsymbol{q}_j$$

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Věta

Nechť $A \in \mathbb{R}^{m,n}, m \geq n$ je libovolná matice. Pak existuje ortogonální matice $Q \in \mathbb{R}^{m,n}$ a horní trojúhelníková matice $R \in \mathbb{R}^{n,n}$ takové, že platí

$$A = QR.$$

- Uvažujme $m = n$. Pak A $=$ QR lze rozepsat jako

$$
(\boldsymbol{a}_1 | \boldsymbol{a}_2 | \cdots | \boldsymbol{a}_n) = (\boldsymbol{q}_1 | \boldsymbol{q}_2 | \cdots | \boldsymbol{q}_n) \begin{pmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,n} \\ & r_{2,2} & & \vdots \\ & & \ddots & \\ 0 & & & r_{n,n} \end{pmatrix}
$$

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$$\left(\boldsymbol{a}_1|\boldsymbol{a}_2|\cdots|\boldsymbol{a}_n\right) = \left(\boldsymbol{q}_1|\boldsymbol{q}_2|\cdots|\boldsymbol{q}_n\right)\begin{pmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,n} \\ & r_{2,2} & & \vdots \\ & & \ddots & \\ 0 & & & r_{n,n} \end{pmatrix}$$

$$\begin{aligned} \boldsymbol{a}_1 &= r_{1,1}\boldsymbol{q}_1 \\ \boldsymbol{a}_2 &= r_{1,2}\boldsymbol{q}_1 + r_{2,2}\boldsymbol{q}_2 \\ &\vdots \\ \boldsymbol{a}_n &= r_{1,n}\boldsymbol{q}_1 + r_{2,n}\boldsymbol{q}_2 + \cdots + r_{n,n}\boldsymbol{q}_n \end{aligned}$$

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$$\begin{aligned} \langle \boldsymbol{a}_1 \rangle &= \langle \boldsymbol{q}_1 \rangle \\ \langle \boldsymbol{a}_1, \boldsymbol{a}_2 \rangle &= \langle \boldsymbol{q}_1, \boldsymbol{q}_2 \rangle \\ &\vdots \\ \langle \boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \rangle &= \langle \boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n \rangle \end{aligned}$$

- Př.

$$\mathsf{A}\boldsymbol{x} = \boldsymbol{b} \quad \Leftrightarrow \quad \underbrace{x_1\boldsymbol{a}_1 + x_2\boldsymbol{a}_2 + \cdots + x_n\boldsymbol{a}_n = \boldsymbol{b}}_{\text{Hledáme koeficienty rozvoje } \boldsymbol{b} \text{ v bázi tvořené sloupci } \mathsf{A}}$$

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- Pokud $\mathsf{A} = \mathsf{QR}$:

$$\mathsf{Q}\underbrace{\mathsf{R}\boldsymbol{x}}_{=\boldsymbol{y}} = \boldsymbol{b}$$

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$$y_k = \boldsymbol{q}_k^T\boldsymbol{b} \quad \to \quad \boldsymbol{y} = \mathsf{Q}^T\boldsymbol{b}$$

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$$\mathsf{R}\boldsymbol{x} = \boldsymbol{y}$$

- Existuje několik způsobů výpočtu
  - pomocí Gramova-Schmidtova procesu,
  - pomocí Givensových rotací,
  - pomocí Householderových transformací.

QR rozklad pomocí Gramova-Schmidtova procesu

- Gramův-Schmidtův proces
  - vstup: nezávislé vektory $\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n$
  - výstup: ortornormální vektory $\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n$ takové, že $\langle \boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n \rangle = \langle \boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n \rangle$

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- První krok: $\boldsymbol{v}_1 = \boldsymbol{a}_1, \boldsymbol{q}_1 = \frac{\boldsymbol{v}_1}{\|\boldsymbol{v}_1\|}, r_{11} = \|\boldsymbol{v}_1\|$

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- Vektor $\boldsymbol{a}_j$ můžeme vyjádřit jako

$$\boldsymbol{a}_j = r_{1,j}\boldsymbol{q}_1 + \cdots + r_{i,j}\boldsymbol{q}_i + \cdots + r_{j-1,j}\boldsymbol{q}_{j-1} + \underbrace{r_{j,j}\boldsymbol{q}_j}_{\overset{\text{ozn.}}{=} \boldsymbol{v}_j}$$

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$$\Downarrow$$

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- $\boldsymbol{v}_j$ má být ortogonální ke známým vektorům $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_{j-1}$, takže pro $k = 1, \ldots, j-1$ musí platit:

$$0 = (\boldsymbol{q}_k, \boldsymbol{v}_j) = (\boldsymbol{q}_k, \boldsymbol{a}_j - r_{1,j}\boldsymbol{q}_1 - \cdots - r_{i,j}\boldsymbol{q}_i - \cdots - r_{j-1,j}\boldsymbol{q}_{j-1})$$

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$$(\boldsymbol{q}_k, \boldsymbol{a}_j - r_{k,j}\boldsymbol{q}_k) = (\boldsymbol{q}_k, \boldsymbol{a}_j) - r_{k,j}\underbrace{(\boldsymbol{q}_k, \boldsymbol{q}_k)}_{=1} = 0$$

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- Získali jsme tedy $\boldsymbol{v}_j$ jako příslušnou lineární kombinaci. Snadno určíme $\boldsymbol{q}_j$ a $r_{j,j}$:

$$\boldsymbol{q}_j = \frac{\boldsymbol{v}_j}{\|\boldsymbol{v}_j\|} = \frac{\boldsymbol{v}_j}{r_{j,j}} \Rightarrow r_{j,j} = \|\boldsymbol{v}_j\|$$

function QR_GS($A \in \mathbb{R}^{m\times n}$)
    $\mathsf{Q} = \mathsf{O} \in \mathbb{R}^{m\times n}$, $\mathsf{R} = \mathsf{O} \in \mathbb{R}^{n\times n}$
    for $j = 1 : n$ **do**
        $\boldsymbol{v} = \mathsf{A}(:, j)$
        for $i = 1, \ldots, j-1$ **do**
            $\mathsf{R}(i, j) = \mathsf{Q}(:, i)^T \mathsf{A}(:, j)$
            $\boldsymbol{v} = \boldsymbol{v} - \mathsf{R}(i, j)\mathsf{Q}(:, i)$
        end for
        $\mathsf{R}(j, j) = \|\boldsymbol{v}\|$
        $\mathsf{Q}(:, j) = \boldsymbol{v}/\mathsf{R}(j, j)$
    end for
end function

function QR_GS($A \in \mathbb{R}^{m\times n}$)
    Q = O $\in \mathbb{R}^{m\times n}$, R = O $\in \mathbb{R}^{n\times n}$
    for $j = 1 : n$ **do**
        $\boldsymbol{v}$ = A(:, j)
        for $i = 1, \dots, j-1$ **do**
            R(i, j) = Q(:, i)^{T}A(:, j)
            $\boldsymbol{v} = \boldsymbol{v}$ − R(i, j)Q(:, i)
        end for
        R(j, j) = $\|\boldsymbol{v}\|$
        Q(:, j) = $\boldsymbol{v}$/R(j, j)
    end for
end function

- Algoritmus vyžaduje $2mn^2$ operací.
- Gramův-Schmidtův proces je numericky nestabilní, v praxi se proto spíše používají Givensovy rotace nebo Householderovy transformace

- Př. Pomocí Gramova-Schmidtova procesu nalezněme QR rozklad matice

$$A = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

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- Hledáme $(\boldsymbol{a}_1 \mid \boldsymbol{a}_2) = (\boldsymbol{q}_1 \mid \boldsymbol{q}_2) \begin{pmatrix} r_{1,1} & r_{1,2} \\ 0 & r_{2,2} \end{pmatrix}$

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$$\begin{aligned} \boldsymbol{v}_1 = &\quad \boldsymbol{a}_1 = \begin{pmatrix} 2 \\ 0 \\ 4 \end{pmatrix}, \|\boldsymbol{v}\| = \sqrt{4+16} = \\ = &\quad \sqrt{20} = 2\sqrt{5} = r_{1,1}, \end{aligned}$$

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$$\boldsymbol{a}_2 = r_{1,2}\boldsymbol{q}_1 + \underbrace{r_{2,2}\boldsymbol{q}_2}_{=\boldsymbol{v}_2} \Rightarrow \boldsymbol{v}_2 = \boldsymbol{a}_2 - r_{1,2}\boldsymbol{q}_1$$

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$$\mathsf{A} = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

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$$\begin{aligned} \boldsymbol{v}_1 = {} & \boldsymbol{a}_1 = \begin{pmatrix} 2 \\ 0 \\ 4 \end{pmatrix}, \|\boldsymbol{v}\| = \sqrt{4+16} = \\ = {} & \sqrt{20} = 2\sqrt{5} = r_{1,1}, \boldsymbol{q}_1 = \begin{pmatrix} 2/2\sqrt{5} \\ 0 \\ 4/2\sqrt{5} \end{pmatrix} = \begin{pmatrix} \sqrt{5}/5 \\ 0 \\ 2\sqrt{5}/5 \end{pmatrix} \end{aligned}$$

$$\boldsymbol{a}_2 = r_{1,2}\boldsymbol{q}_1 + \underbrace{r_{2,2}\boldsymbol{q}_2}_{=\boldsymbol{v}_2} \Rightarrow \boldsymbol{v}_2 = \boldsymbol{a}_2 - r_{1,2}\boldsymbol{q}_1$$

$$0 = \boldsymbol{q}_1^T \boldsymbol{v}_2 = \boldsymbol{q}_1^T \boldsymbol{a}_2 - r_{1,2}\boldsymbol{q}_1^T \boldsymbol{q}_1$$

- Př. Pomocí Gramova-Schmidtova procesu nalezněme QR rozklad matice
$$\mathsf{A} = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

- Hledáme $(\boldsymbol{a}_1 \mid \boldsymbol{a}_2) = (\boldsymbol{q}_1 \mid \boldsymbol{q}_2) \begin{pmatrix} r_{1,1} & r_{1,2} \\ 0 & r_{2,2} \end{pmatrix}$

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$$\Rightarrow r_{1,2} = \boldsymbol{q}_1^T \boldsymbol{a}_2 = \frac{\sqrt{5}}{5} \cdot 3 + 0 \cdot 1 + \frac{2\sqrt{5}}{5} \cdot 1 = \sqrt{5}$$

- Př. Pomocí Gramova-Schmidtova procesu nalezněme QR rozklad matice

$$\mathsf{A} = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

- Hledáme $(\boldsymbol{a}_1 \,|\, \boldsymbol{a}_2) = (\boldsymbol{q}_1 \,|\, \boldsymbol{q}_2) \begin{pmatrix} r_{1,1} & r_{1,2} \\ 0 & r_{2,2} \end{pmatrix}$

$$\begin{aligned} \boldsymbol{v}_1 = &\quad \boldsymbol{a}_1 = \begin{pmatrix} 2 \\ 0 \\ 4 \end{pmatrix}, \|\boldsymbol{v}\| = \sqrt{4+16} = \\ = &\quad \sqrt{20} = 2\sqrt{5} = r_{1,1}, \boldsymbol{q}_1 = \begin{pmatrix} 2/2\sqrt{5} \\ 0 \\ 4/2\sqrt{5} \end{pmatrix} = \begin{pmatrix} \sqrt{5}/5 \\ 0 \\ 2\sqrt{5}/5 \end{pmatrix} \end{aligned}$$

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$$\Rightarrow r_{1,2} = \boldsymbol{q}_1^T \boldsymbol{a}_2 = \frac{\sqrt{5}}{5} \cdot 3 + 0 \cdot 1 + \frac{2\sqrt{5}}{5} \cdot 1 = \sqrt{5}$$

$$\boldsymbol{v}_2 = \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix} - \sqrt{5} \begin{pmatrix} \sqrt{5}/5 \\ 0 \\ 2\sqrt{5}/5 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ -1 \end{pmatrix}$$

- Př. Pomocí Gramova-Schmidtova procesu nalezněme QR rozklad matice

$$\mathsf{A} = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

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$$\begin{aligned} \boldsymbol{v}_1 = \quad & \boldsymbol{a}_1 = \begin{pmatrix} 2 \\ 0 \\ 4 \end{pmatrix}, \|\boldsymbol{v}\| = \sqrt{4+16} = \\ = \quad & \sqrt{20} = 2\sqrt{5} = r_{1,1}, \boldsymbol{q}_1 = \begin{pmatrix} 2/2\sqrt{5} \\ 0 \\ 4/2\sqrt{5} \end{pmatrix} = \begin{pmatrix} \sqrt{5}/5 \\ 0 \\ 2\sqrt{5}/5 \end{pmatrix} \end{aligned}$$

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$$\|\boldsymbol{v}_2\| = \sqrt{2^2+1+1} = \sqrt{6} = r_{2,2}$$

- Př. Pomocí Gramova-Schmidtova procesu nalezněme QR rozklad matice

$$A = \begin{pmatrix} 2 & 3 \\ 0 & 1 \\ 4 & 1 \end{pmatrix}$$

- Hledáme $(\boldsymbol{a}_1 \mid \boldsymbol{a}_2) = (\boldsymbol{q}_1 \mid \boldsymbol{q}_2) \begin{pmatrix} r_{1,1} & r_{1,2} \\ 0 & r_{2,2} \end{pmatrix}$

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$$\boldsymbol{a}_2 = r_{1,2}\boldsymbol{q}_1 + \underbrace{r_{2,2}\boldsymbol{q}_2}_{=\boldsymbol{v}_2} \Rightarrow \boldsymbol{v}_2 = \boldsymbol{a}_2 - r_{1,2}\boldsymbol{q}_1$$

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$$\boldsymbol{q}_2 = \boldsymbol{v}_2 / \|\boldsymbol{v}_2\| = \begin{pmatrix} \sqrt{6}/3 \\ \sqrt{6}/6 \\ -\sqrt{6}/6 \end{pmatrix}$$

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$$\mathsf{Q} = \begin{pmatrix} \sqrt{5}/5 & \sqrt{6}/3 \\ 0 & \sqrt{6}/6 \\ 2\sqrt{5}/5 & -\sqrt{6}/6 \end{pmatrix}, \mathsf{R} = \begin{pmatrix} 2\sqrt{5} & \sqrt{5} \\ 0 & \sqrt{6} \end{pmatrix}$$

Redukovaná vs. plná QR faktorizace

- Redukovaná QR faktorizace

$$\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{pmatrix} = \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{pmatrix} \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix}$$

Redukovaná vs. plná QR faktorizace

- Redukovaná QR faktorizace

$$\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{pmatrix} = \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{pmatrix} \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix}$$

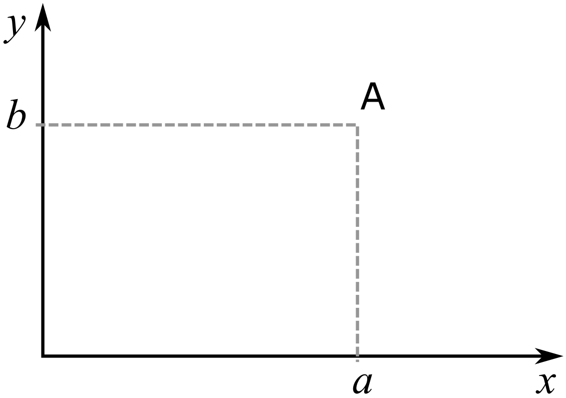
- Plná QR faktorizace

$$\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{pmatrix} = \begin{pmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{pmatrix} \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Givensova transformace

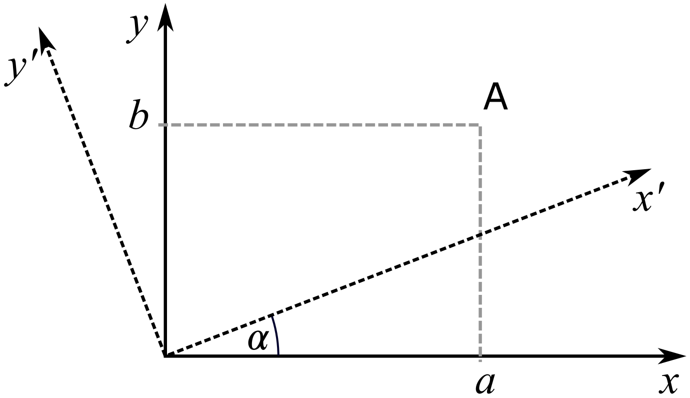
- Uvažujme dva souřadné systémy: xy a $x'y'$

Givensova transformace



- Uvažujme dva souřadné systémy: xy a $x'y'$
- Bod A má souřadnice (a, b) v xy

Givensova transformace



- Uvažujme dva souřadné systémy: xy a $x'y'$
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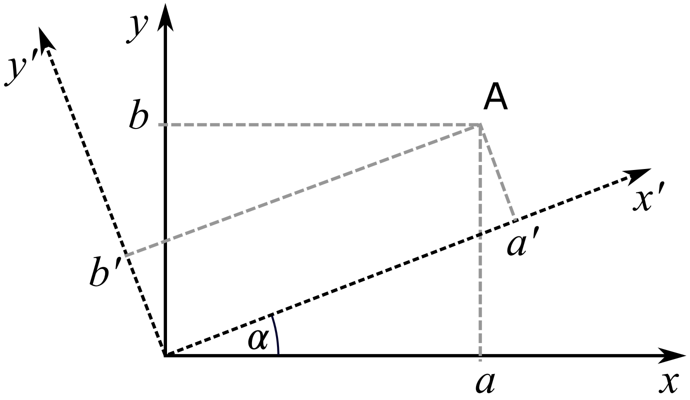
- Vyjádřeme jeho souřadnice v $x'y'$

Givensova transformace



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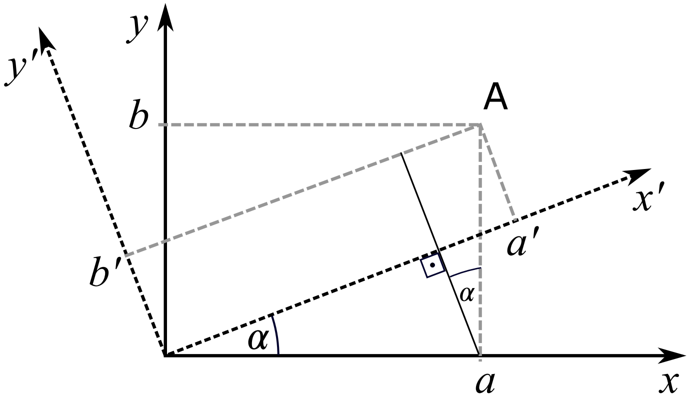

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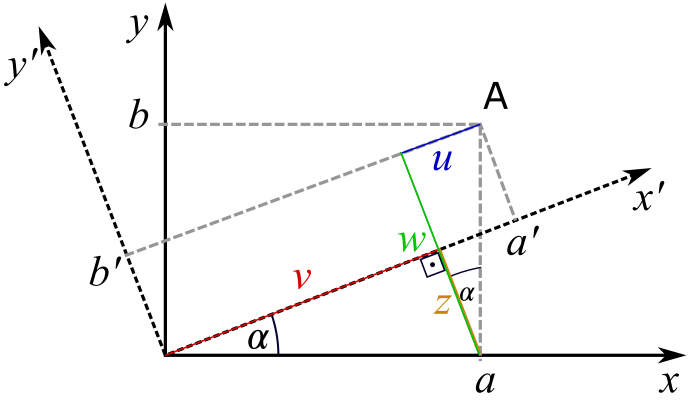

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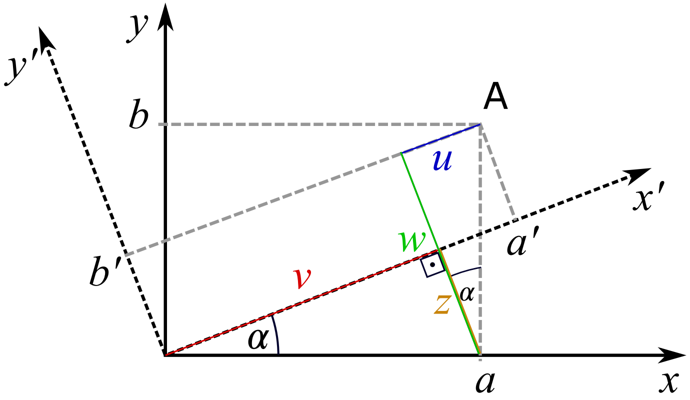
$$\sin\alpha = \frac{u}{b} \Rightarrow u = b\sin\alpha$$

Givensova transformace



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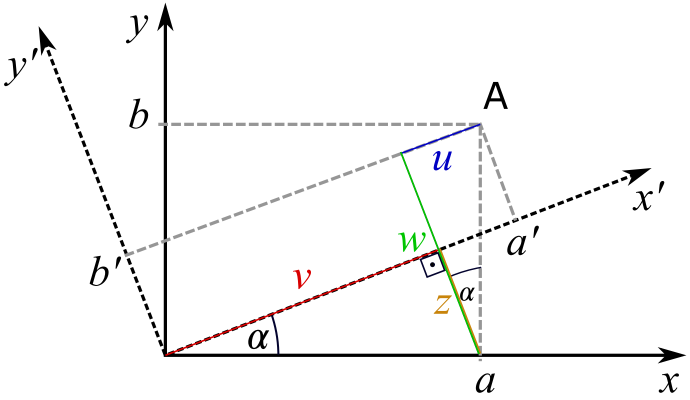
Givensova transformace



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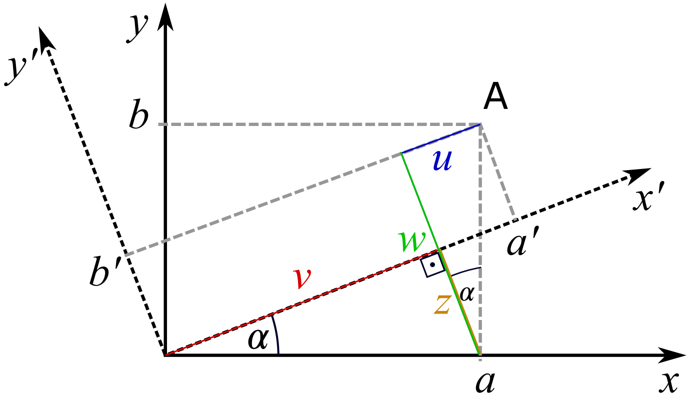
Givensova transformace



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$$\begin{aligned} a' &= \quad a\cos\alpha + b\sin\alpha \\ b' &= \quad -a\sin\alpha + b\cos\alpha \end{aligned}$$

$$\begin{aligned} a' &= \quad a\cos\alpha + b\sin\alpha \\ b' &= \quad -a\sin\alpha + b\cos\alpha \end{aligned} \qquad \begin{pmatrix} a' \\ b' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}_{=\mathsf{G}} \begin{pmatrix} a \\ b \end{pmatrix}$$

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- Matici G nazýváme maticí rovinné rotace, která vektor (a, b) rotuje o úhel $-\alpha$ (rotujeme soustavu souřadnic o úhel $\alpha \Leftrightarrow$ rotujeme vektor o úhel $-\alpha$)

$$\begin{aligned} a' &= \quad a\cos\alpha + b\sin\alpha \\ b' &= \quad -a\sin\alpha + b\cos\alpha \end{aligned} \qquad \begin{pmatrix} a' \\ b' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}_{=\mathsf{G}} \begin{pmatrix} a \\ b \end{pmatrix}$$

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- Matice G je otrogonální, $\mathsf{G}^{-1} = \mathsf{G}^T$ rotuje vektor o úhel α

$$\begin{aligned} a' &= \quad a\cos\alpha + b\sin\alpha \\ b' &= \quad -a\sin\alpha + b\cos\alpha \end{aligned} \qquad \begin{pmatrix} a' \\ b' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}_{=\mathsf{G}} \begin{pmatrix} a \\ b \end{pmatrix}$$

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- Označme $c = \cos\alpha, s = \sin\alpha$
- Matici rotace je možné využít k nulování prvků vektoru, např.

$$\mathsf{G}^T \boldsymbol{x} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sqrt{a^2 + b^2} \\ 0 \end{pmatrix}$$

$$\begin{aligned} a' &= \quad a\cos\alpha + b\sin\alpha \\ b' &= \quad -a\sin\alpha + b\cos\alpha \end{aligned} \qquad \begin{pmatrix} a' \\ b' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}}_{=\mathsf{G}} \begin{pmatrix} a \\ b \end{pmatrix}$$

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$$\begin{aligned} ac - bs &= \quad \sqrt{a^2 + b^2} \\ as + bc &= \quad 0 \end{aligned}$$

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$$\begin{aligned} ac - bs &= \quad \sqrt{a^2 + b^2} \\ as + bc &= \quad 0 \end{aligned} \quad \Rightarrow c = \frac{a}{\sqrt{a^2 + b^2}}, \quad s = -\frac{b}{\sqrt{a^2 + b^2}}$$

- Postup lze zobecnit i pro vektory délky n:

$$\mathsf{G}_{i,j} = \begin{pmatrix} 1 & & & \cdots & & & 0 \\ & \ddots & & & & & \\ & & c & & s & & \\ \vdots & & & \ddots & & & \vdots \\ & & -s & & c & & \\ & & & & & \ddots & \\ 0 & & & \cdots & & & 1 \end{pmatrix}$$

- Postup lze zobecnit i pro vektory délky n:

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- i, j - osy, ve kterých se rotuje

- Postup lze zobecnit i pro vektory délky n:

$$\mathsf{G}_{i,j} = \begin{pmatrix} 1 & & & \cdots & & & 0 \\ & \ddots & & & & & \\ & & c & & s & & \\ \vdots & & & \ddots & & & \vdots \\ & & -s & & c & & \\ & & & & & \ddots & \\ 0 & & & \cdots & & & 1 \end{pmatrix}$$

- i, j - osy, ve kterých se rotuje

$$\boldsymbol{y} = \mathsf{G}_{i,j}^T \boldsymbol{x}$$

$$y_k = \begin{cases} cx_i - sx_j, & k = i, \\ sx_i + cx_j, & k = j, \\ x_k, & k \neq i, j, \end{cases}$$

- Postup lze zobecnit i pro vektory délky n:

$$\mathsf{G}_{i,j} = \begin{pmatrix} 1 & & & \cdots & & & 0 \\ & \ddots & & & & & \\ & & c & & s & & \\ \vdots & & & \ddots & & & \vdots \\ & & -s & & c & & \\ & & & & & \ddots & \\ 0 & & & \cdots & & & 1 \end{pmatrix}$$

- i, j - osy, ve kterých se rotuje

$$\boldsymbol{y} = \mathsf{G}_{i,j}^T \boldsymbol{x}$$

$$y_k = \begin{cases} cx_i - sx_j, & k = i, \\ sx_i + cx_j, & k = j, \\ x_k, & k \neq i, j, \end{cases} \qquad c = \frac{x_i}{\sqrt{x_i^2 + x_j^2}}, \quad s = \frac{-x_j}{\sqrt{x_i^2 + x_j^2}}.$$

- Givensova QR metoda:

$$\mathsf{G}(i-1,i)=\mathsf{G}_{i-1,i},\quad c=\frac{x_{i-1}}{\sqrt{x_{i-1}^2+x_i^2}},s=\frac{-x_{i-1}}{\sqrt{x_{i-1}^2+x_i^2}}$$

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$$\mathsf{A} = \begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix} \overset{\mathsf{G}(2,3)^T}{\longrightarrow} \begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \end{pmatrix} \overset{\mathsf{G}(1,2)^T}{\longrightarrow} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{pmatrix} \overset{\mathsf{G}(2,3)^T}{\longrightarrow} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{pmatrix}$$

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- Postupně tedy aplikujeme zleva jednotlivé ortogonální transformační matice G_k^T:

$$\underbrace{\mathsf{G}_p^T \mathsf{G}_{p-1}^T \cdots \mathsf{G}_2^T \mathsf{G}_1^T}_{=\mathsf{Q}^T} \mathsf{A} = \mathsf{R}$$

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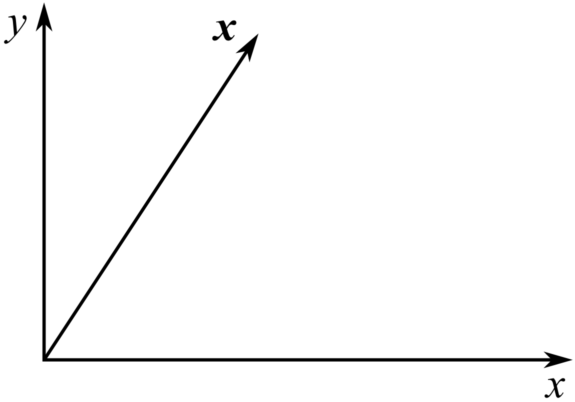
$$\mathsf{A} = \mathsf{G}_1 \mathsf{G}_2 \cdots \mathsf{G}_{p-1} \mathsf{G}_p \mathsf{R}, \quad \mathsf{A} = \mathsf{QR}$$

function QR_Givens($A \in \mathbb{R}^{m\times n}$)
    Q $=$ I $\in \mathbb{R}^{m\times m}$, R $=$ A
    for $j = 1 : n$ **do**
        for $i = m, m-1, \ldots, j+1$ **do**
            $x =$ R$(:, j)$
            if $\sqrt{x_{i-1}^2 + x_i^2} > 0$ **then**
                $c = x_{i-1}/\sqrt{x_{i-1}^2 + x_i^2)}$
                $s = -x_i/\sqrt{x_{i-1}^2 + x_i^2)}$
                G $=$ I $\in \mathbb{R}^{m\times m}$
                G$([i-1, i], [i-1, i]) = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}$
                R $=$ G^{T}R
                Q $=$ QG
            end if
        end for
    end for
end function

- Algoritmus vyžaduje přibližně $3n^2m - n^3$ operací.

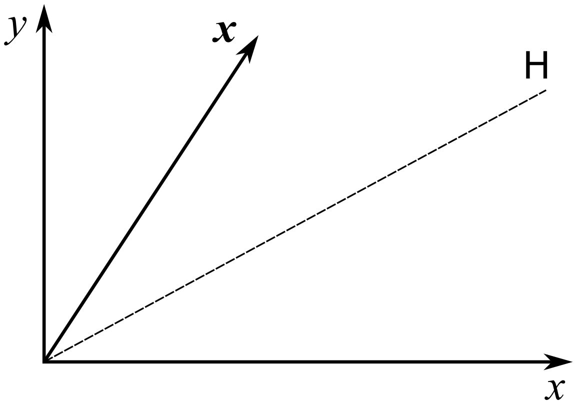
Householderovy transformace



- K vektoru $\boldsymbol{x}$ sestrojíme jeho projekci do osy x stejné délky

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \xrightarrow{\mathsf{P}} \mathsf{P}\boldsymbol{x} = \begin{pmatrix} \|\boldsymbol{x}\| \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \|\boldsymbol{x}\|\boldsymbol{e}_1$$

Householderovy transformace



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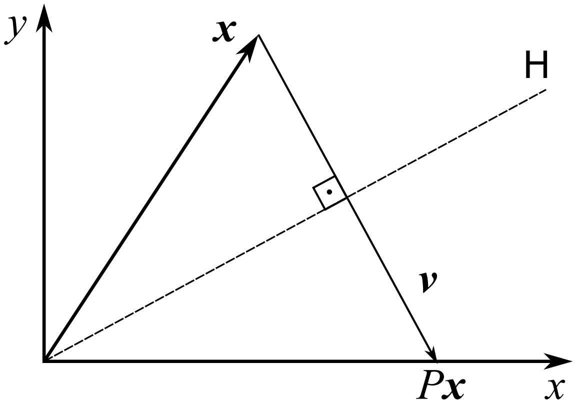

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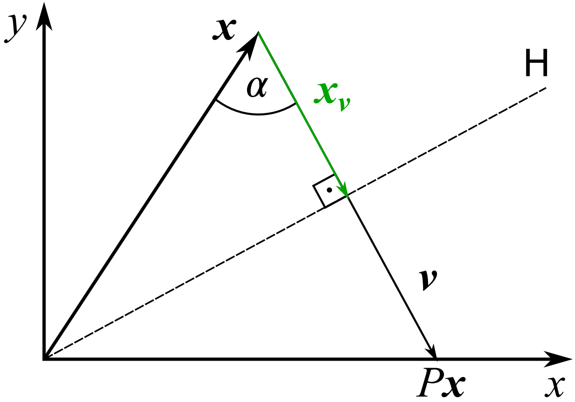
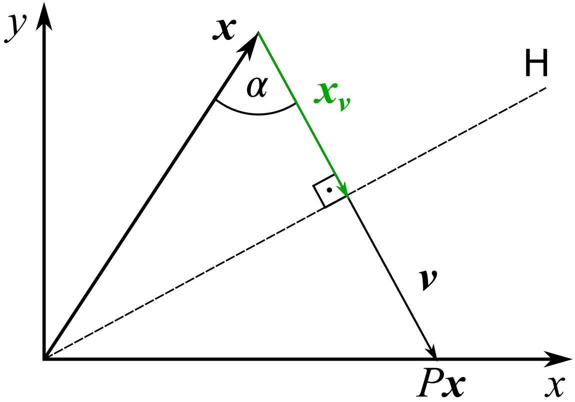


- P$\boldsymbol{x}$ má mít stejnou délku jako $\boldsymbol{x}$, tzn. $\|\mathrm{P}\boldsymbol{x}\| = (\mathrm{P}\boldsymbol{x})_1 = \|\boldsymbol{x}\|$



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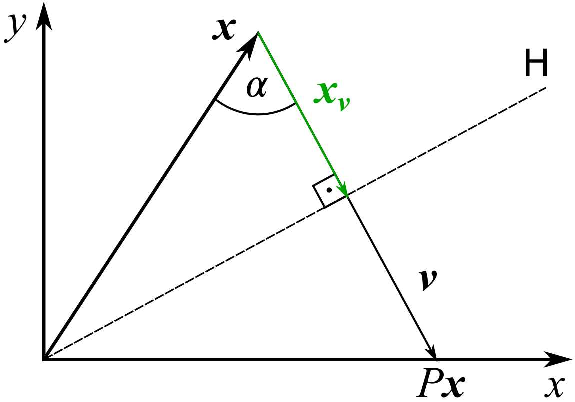
- P$\boldsymbol{x}$ je zrcadlový obraz $\boldsymbol{x}$ s osou souměrnosti H, osa prochází počátkem a je kolmá k $\boldsymbol{v} = \mathsf{P}\boldsymbol{x} - \boldsymbol{x} = \|\boldsymbol{x}\|\boldsymbol{e}_1 - \boldsymbol{x}$



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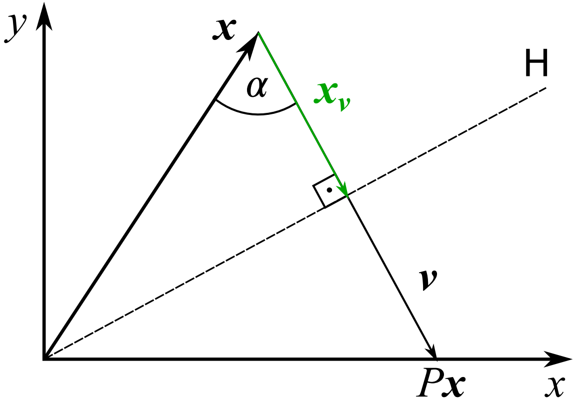
$$\mathsf{P}\boldsymbol{x} = \boldsymbol{x} + 2\boldsymbol{x}_v$$

$$\boldsymbol{x}_v = \boldsymbol{v}_n\|\boldsymbol{x}\|\cos\alpha, \text{ kde } \boldsymbol{v}_n = \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|}$$



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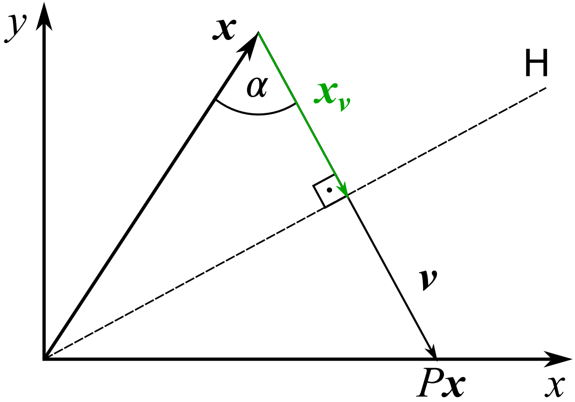

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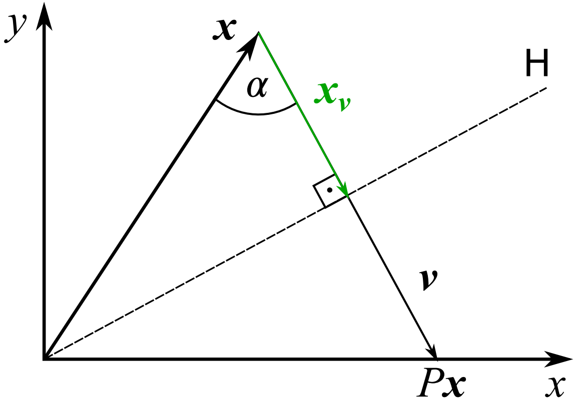
$$\Rightarrow \mathsf{P} = \mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$



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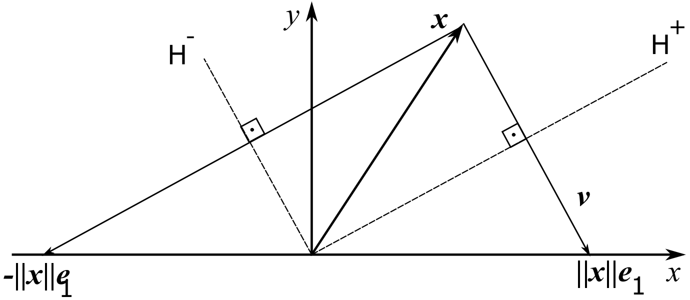
$$\Rightarrow \mathsf{P} = \mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}} \quad \text{matice zrcadlení (Householderova matice)}$$



- Projekce do osy x není definována jednoznačně $(\pm\|\boldsymbol{x}\|\boldsymbol{e}_1)$.
- Pro lepší numerickou stabilitu se volí projekce volí jako $\mathsf{P}\boldsymbol{x} = -\operatorname{sign}(x_1)\boldsymbol{e}_1$

- P je symetrická ortogonální matice:

$$\mathsf{P}^T = (\mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}})^T = \mathsf{I} - 2\frac{(\boldsymbol{v}^T)^T\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}} = \mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$

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$$\mathsf{P}\mathsf{P}^T = \mathsf{P}\mathsf{P} = (\mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}})(\mathsf{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}) = \mathsf{I} - 4\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}} + 4\frac{\boldsymbol{v}\boldsymbol{v}^T\boldsymbol{v}\boldsymbol{v}^T}{(\boldsymbol{v}^T\boldsymbol{v})^2} = \mathsf{I} - 4\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}} + 4\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}} = \mathsf{I}$$

- Householderova QR dekompozice

$$\begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix} \xrightarrow{\mathsf{P}_1} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{pmatrix} \xrightarrow{\mathsf{P}_2} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{pmatrix} \xrightarrow{\mathsf{P}_3} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{pmatrix}$$

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$$\begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix} \xrightarrow{\mathsf{P}_1} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{pmatrix} \xrightarrow{\mathsf{P}_2} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{pmatrix} \xrightarrow{\mathsf{P}_3} \begin{pmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{pmatrix}$$

$$\underbrace{\mathsf{P}_n \mathsf{P}_{n-1} \cdots \mathsf{P}_1}_{=\mathsf{Q}^T} \mathsf{A} = \mathsf{R} \quad \Rightarrow \mathsf{A} = \mathsf{QR}, \mathsf{Q} = \mathsf{P}_1 \cdots \mathsf{P}_{n-1} \mathsf{P}_n$$

function QR_Householder($A \in \mathbb{R}^{m \times n}$)
  Q $=$ I $\in \mathbb{R}^{m \times m}$, R $=$ A
  for $j = 1 : n$ **do**
    $\boldsymbol{x} =$ R$(j : m, j)$
    $\boldsymbol{v} = -\mathrm{sign}(x_1)\|\boldsymbol{x}\|eye(m - j + 1, 1) - \boldsymbol{x}$
    $\boldsymbol{v} = \boldsymbol{v}/\|\boldsymbol{v}\|$
    P $=$ I $\in \mathbb{R}^{m \times m}$
    P$(j : m, j : m) =$ P$(j : m, j : m) - 2\boldsymbol{v}\boldsymbol{v}^T$
    R $=$ PR
    Q $=$ QP
  end for
end function

- Algoritmus vyžaduje přibližně $2mn^2 - \frac{2}{3}n^3$ operací.

- Aplikace QR rozkladu
  - výpočet ortonormální báze z množiny vektorů
  - řešení soustav lineárních rovnic
  - řešení problému nejmenších čtverců (přeurčených soustav)
  - hledání vlastních čísel (spektrální rozklad)
  - výpočet pseudoinverze (Moore-Penroseovy):

$$
\begin{aligned}
\mathsf{A}\mathsf{A}^{+}\mathsf{A} &= \mathsf{A},\\
\mathsf{A}^{+}\mathsf{A}\mathsf{A}^{+} &= \mathsf{A},\\
(\mathsf{A}\mathsf{A}^{+})^{T} &= \mathsf{A}\mathsf{A}^{+}\\
,(\mathsf{A}^{+}\mathsf{A})^{T} &= \mathsf{A}^{+}\mathsf{A}
\end{aligned}
$$

Děkuji za pozornost

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20. dubna 2023

VŠB TECHNICKÁ UNIVERZITA OSTRAVA | IT4INNOVATIONS NÁRODNÍ SUPERPOČÍTAČOVÉ CENTRUM