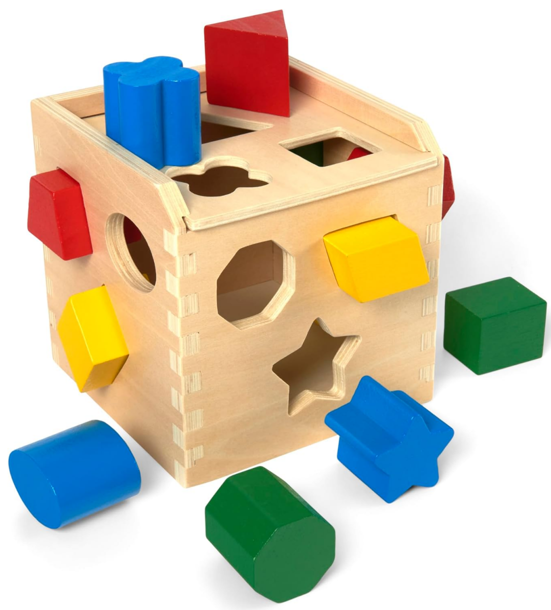
Bedste linje og bedste docking

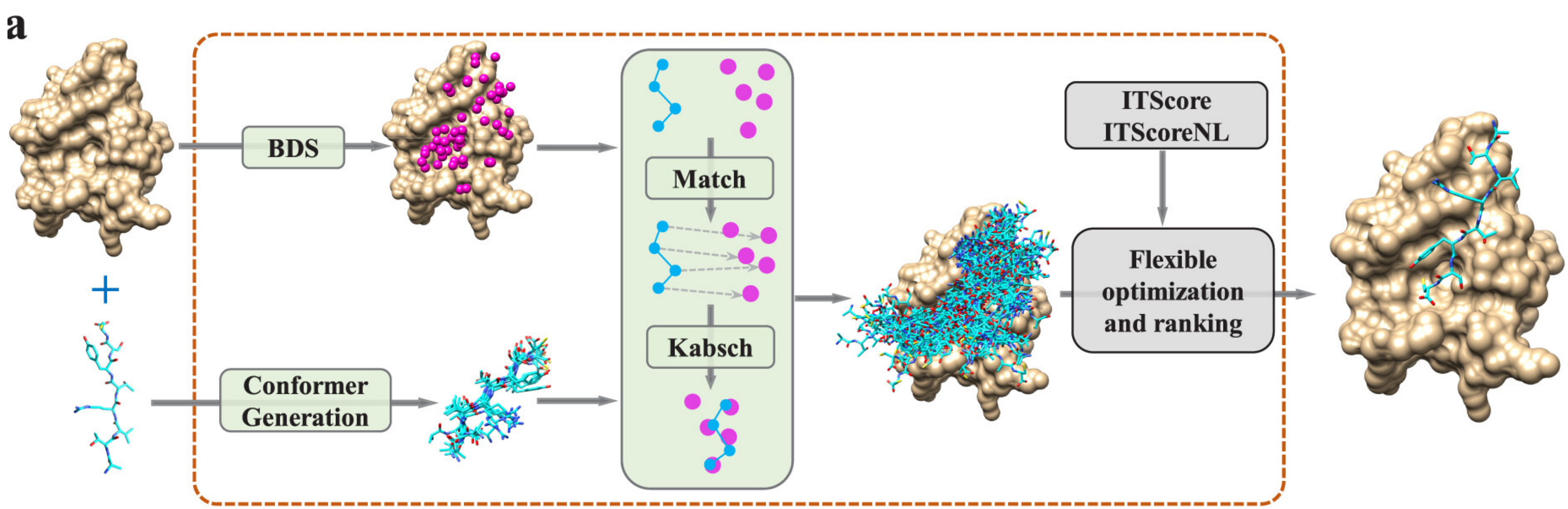
v./ Steen Markvorsen, DTU Compute

IM 2.0 Projektdag, DTU, 15.12.25

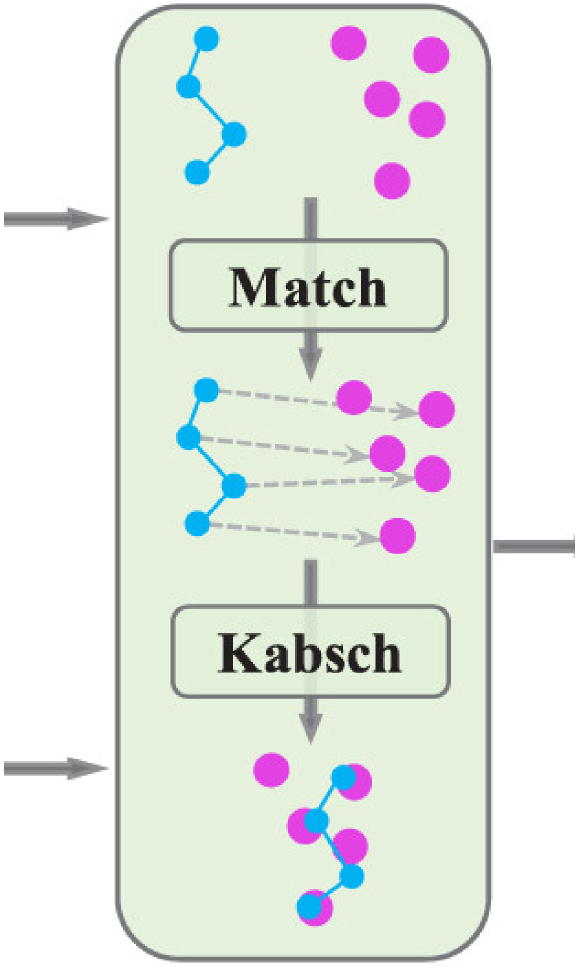
Puttekasse-problemet



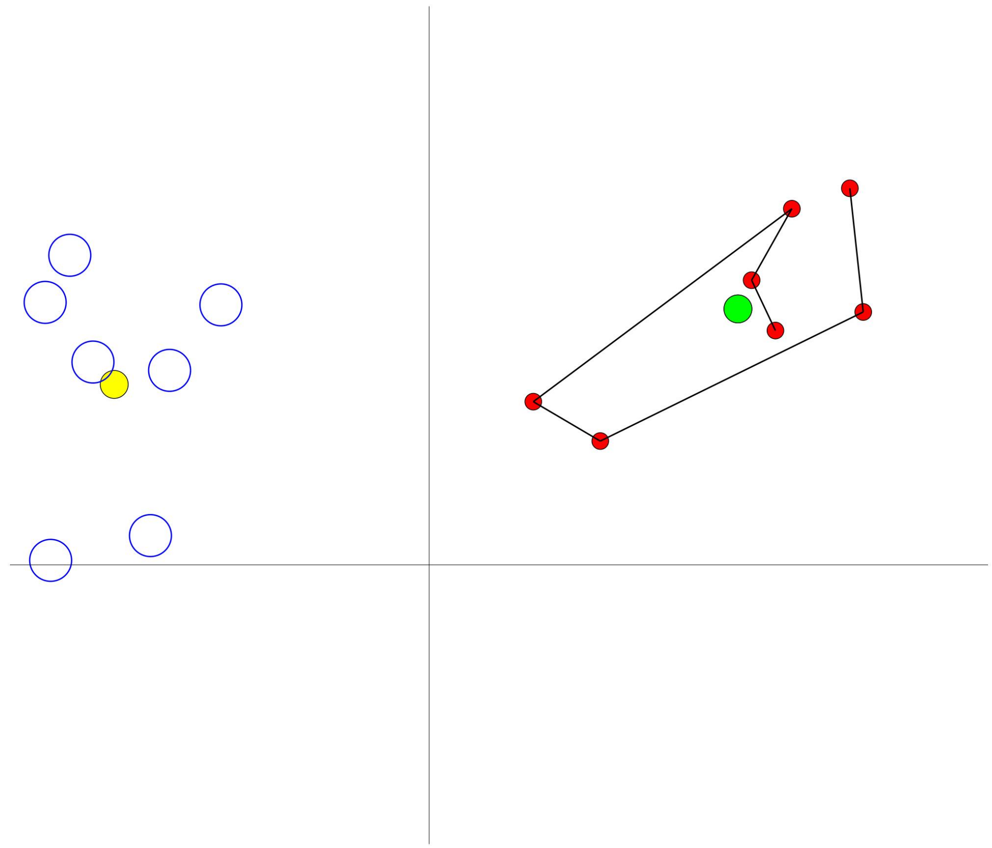
Molekylær docking

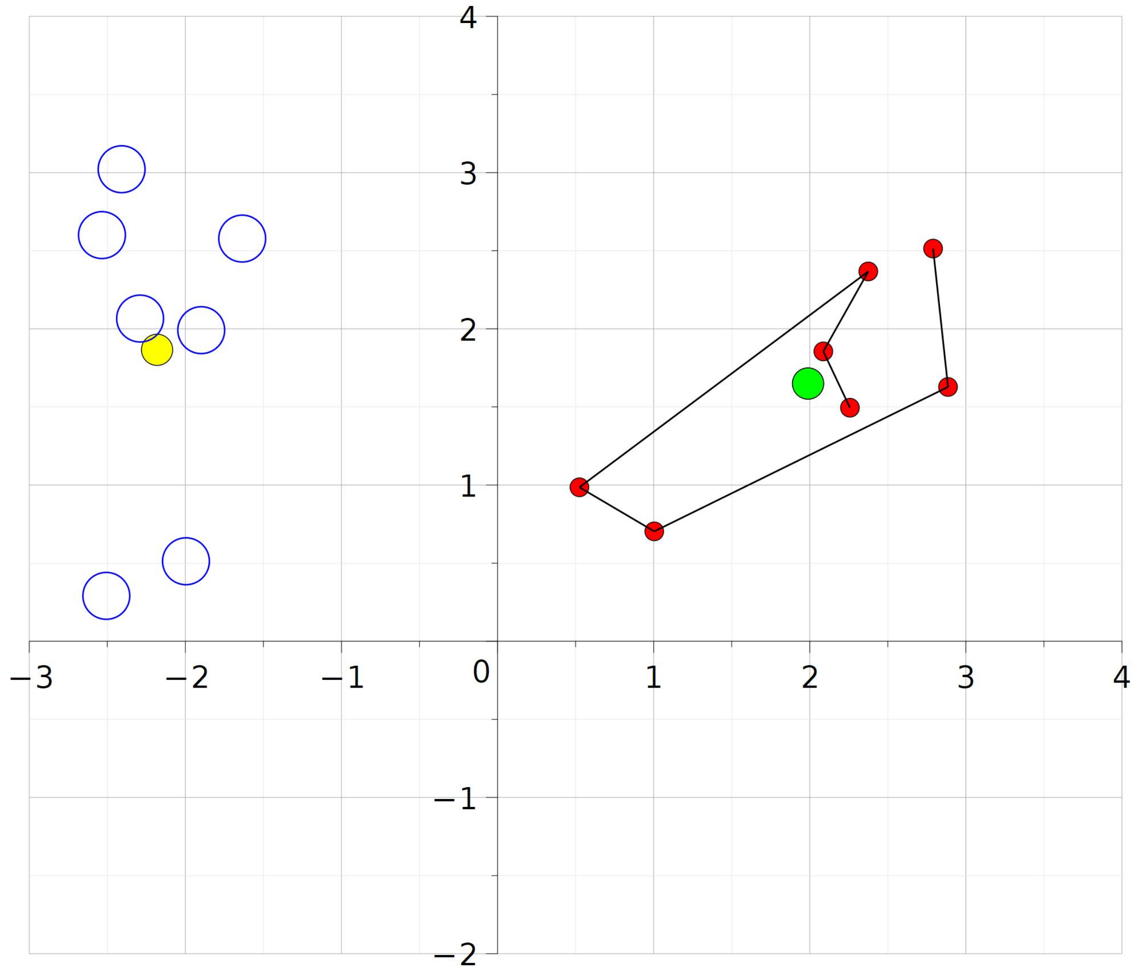


Molekylær docking



Fænomenologisk: Docking i 2D





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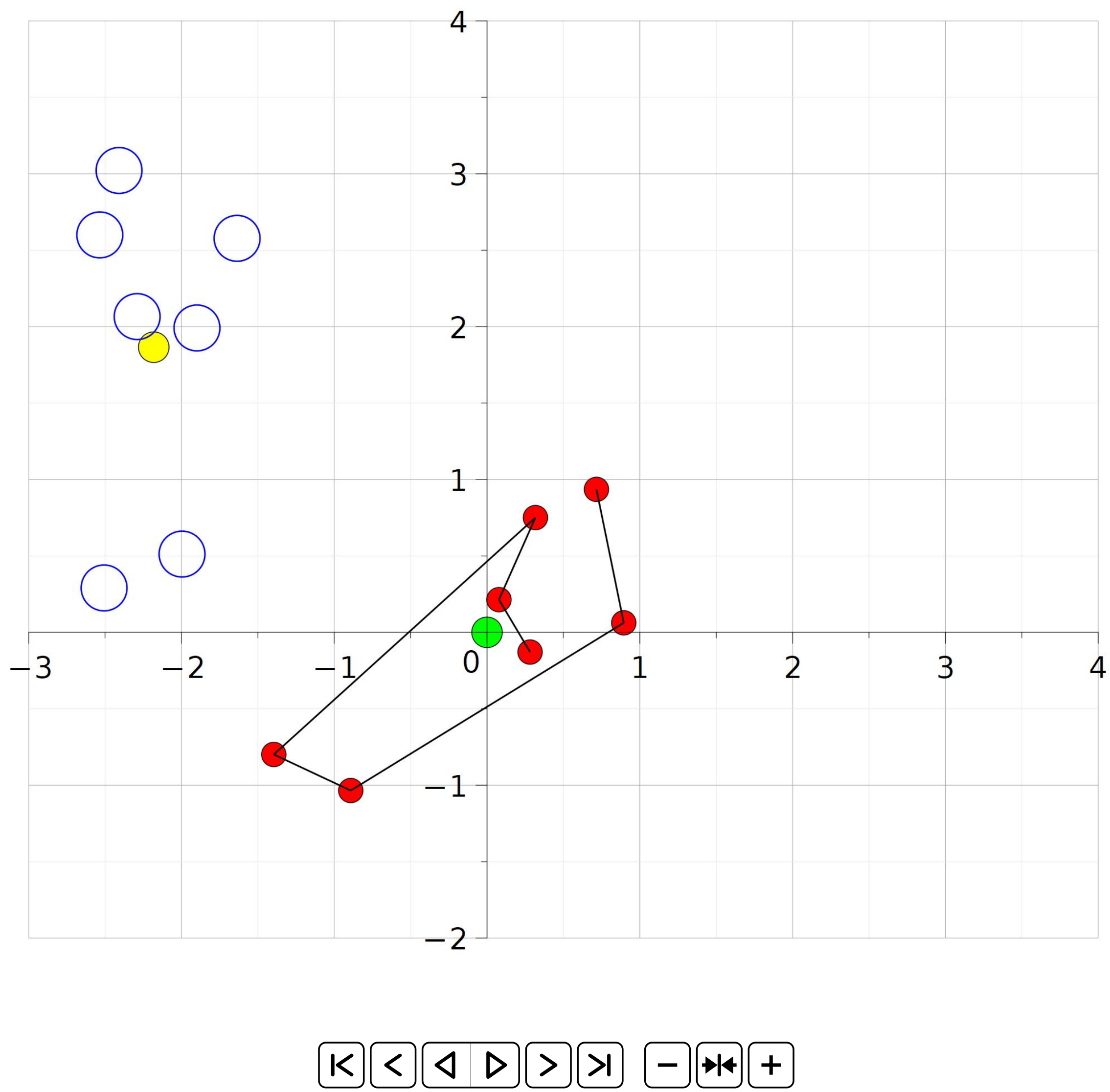
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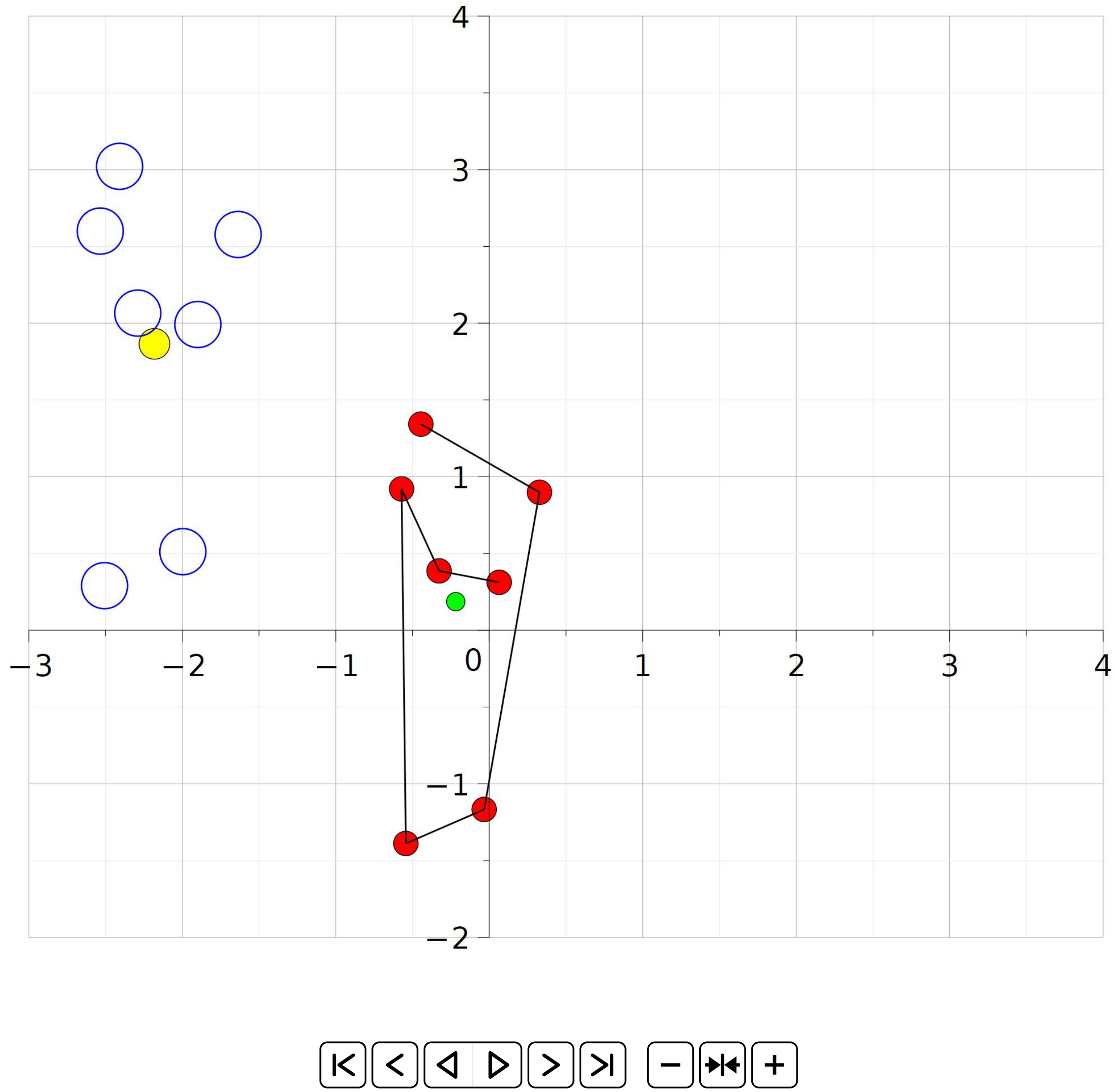
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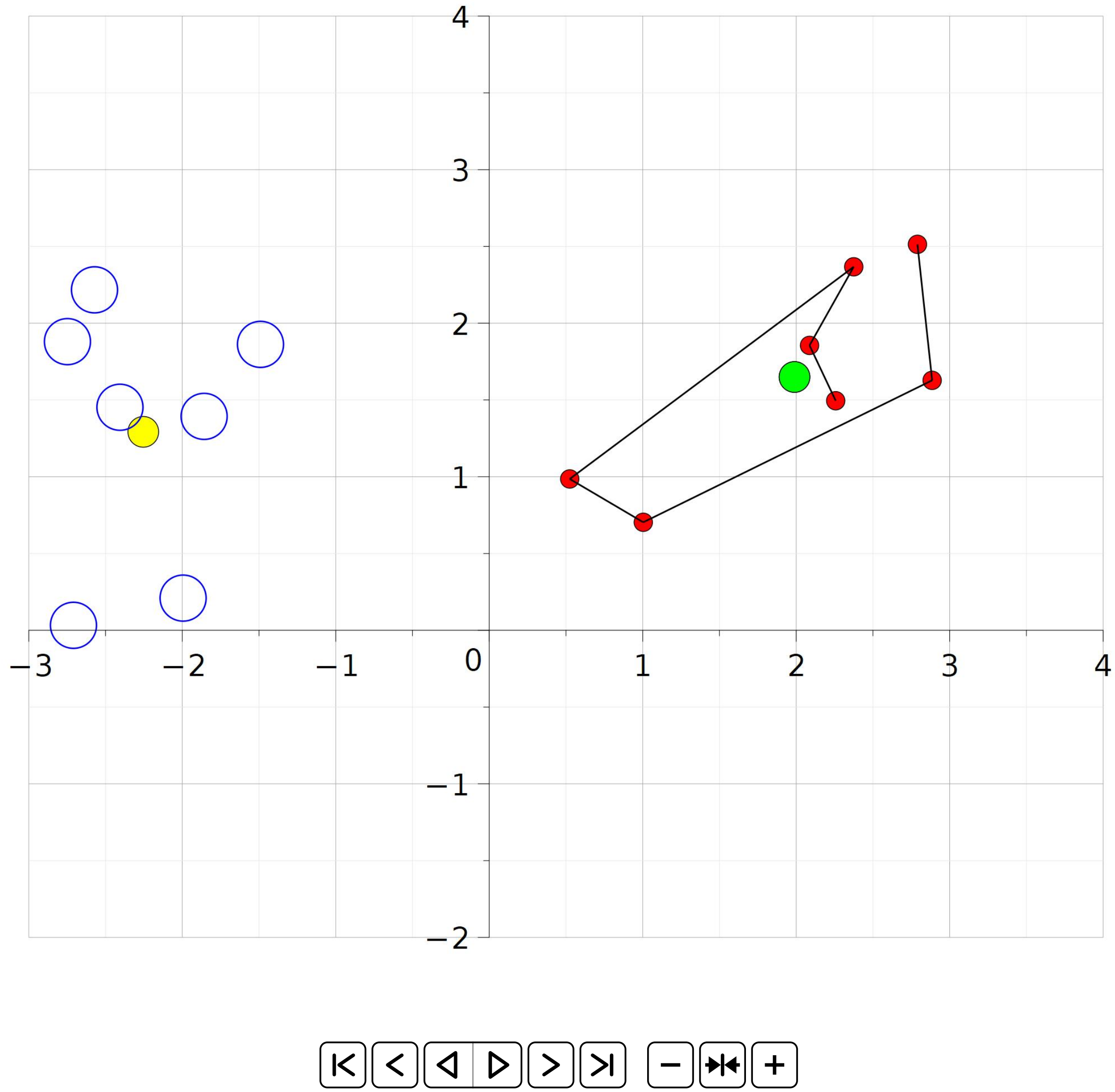
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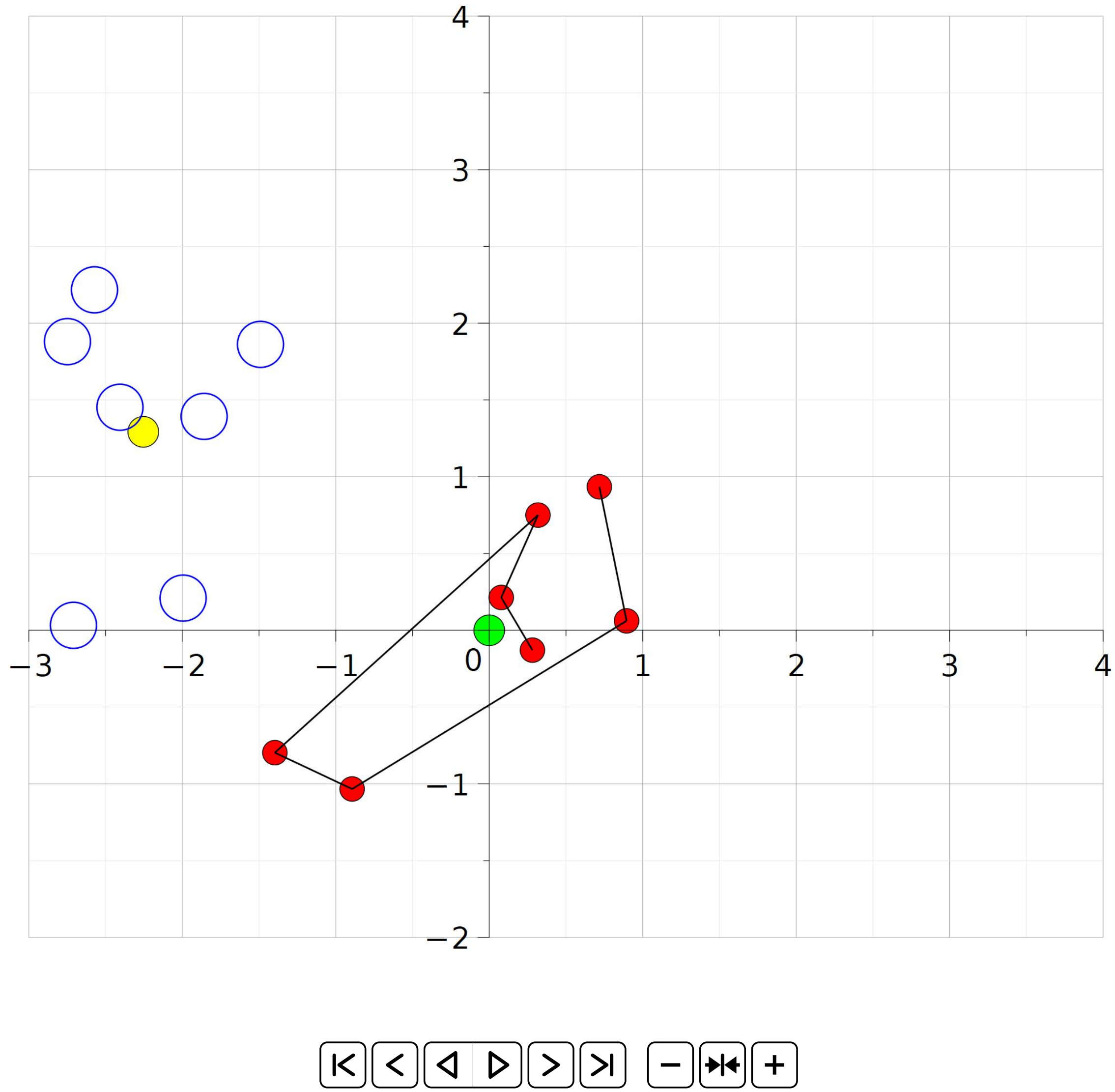

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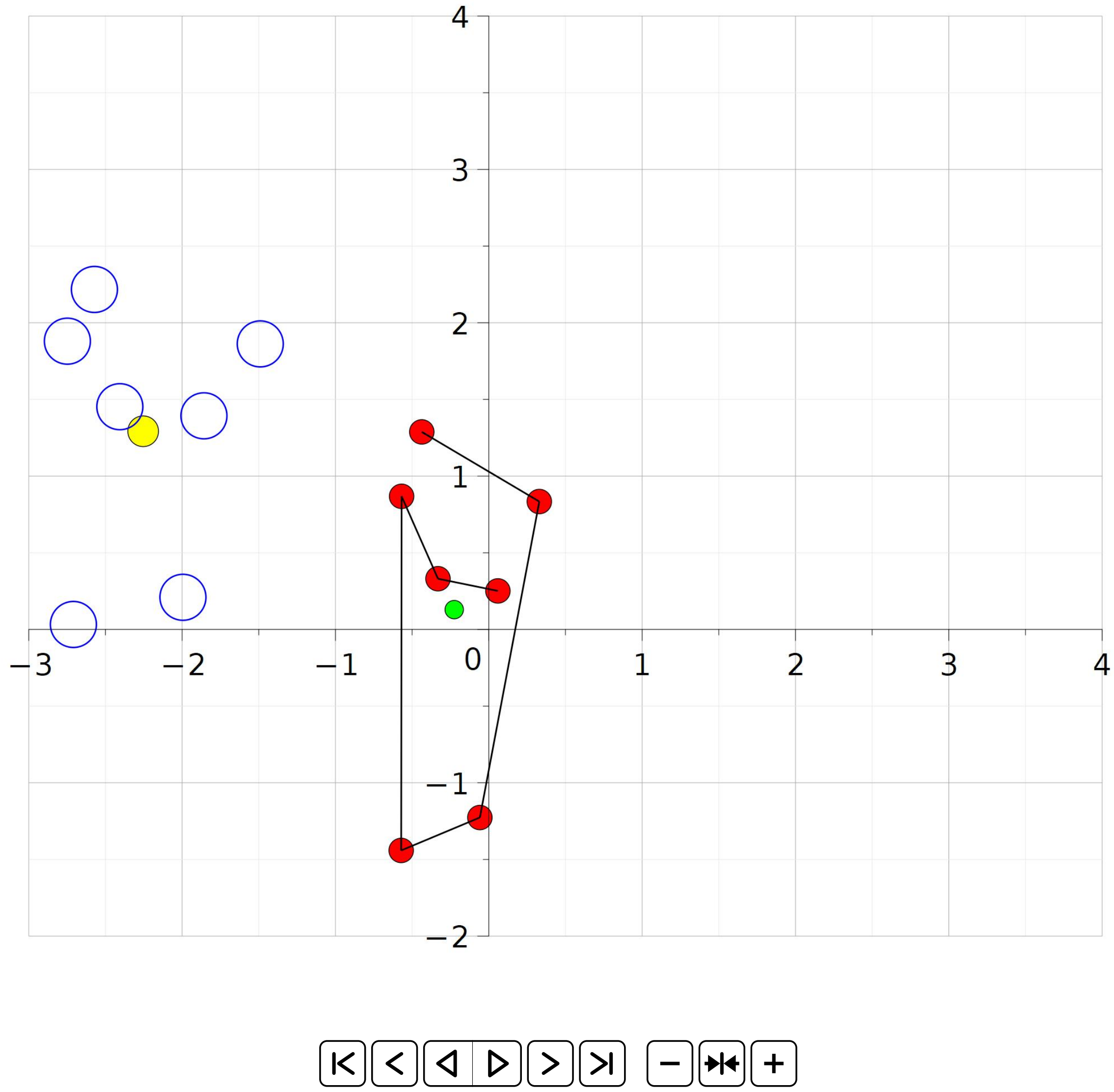

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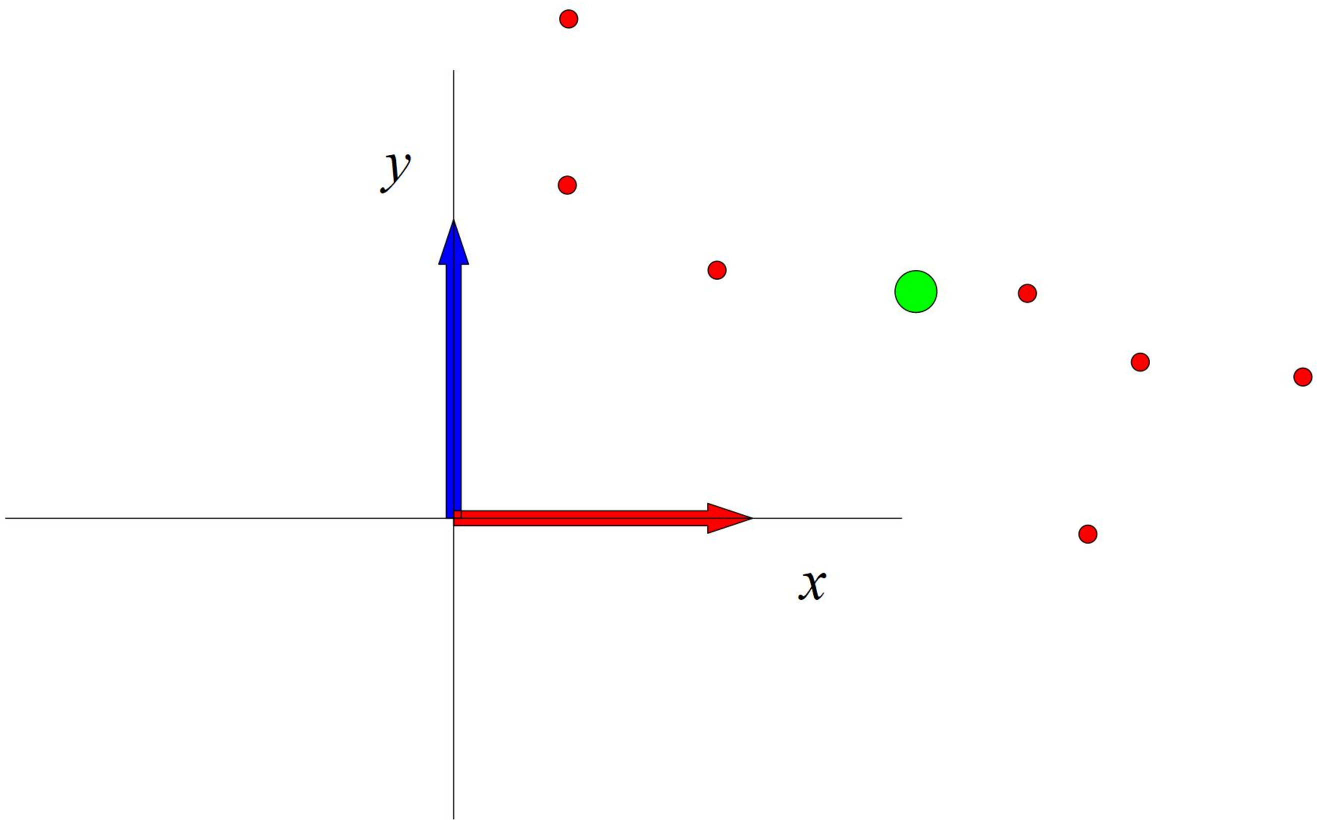
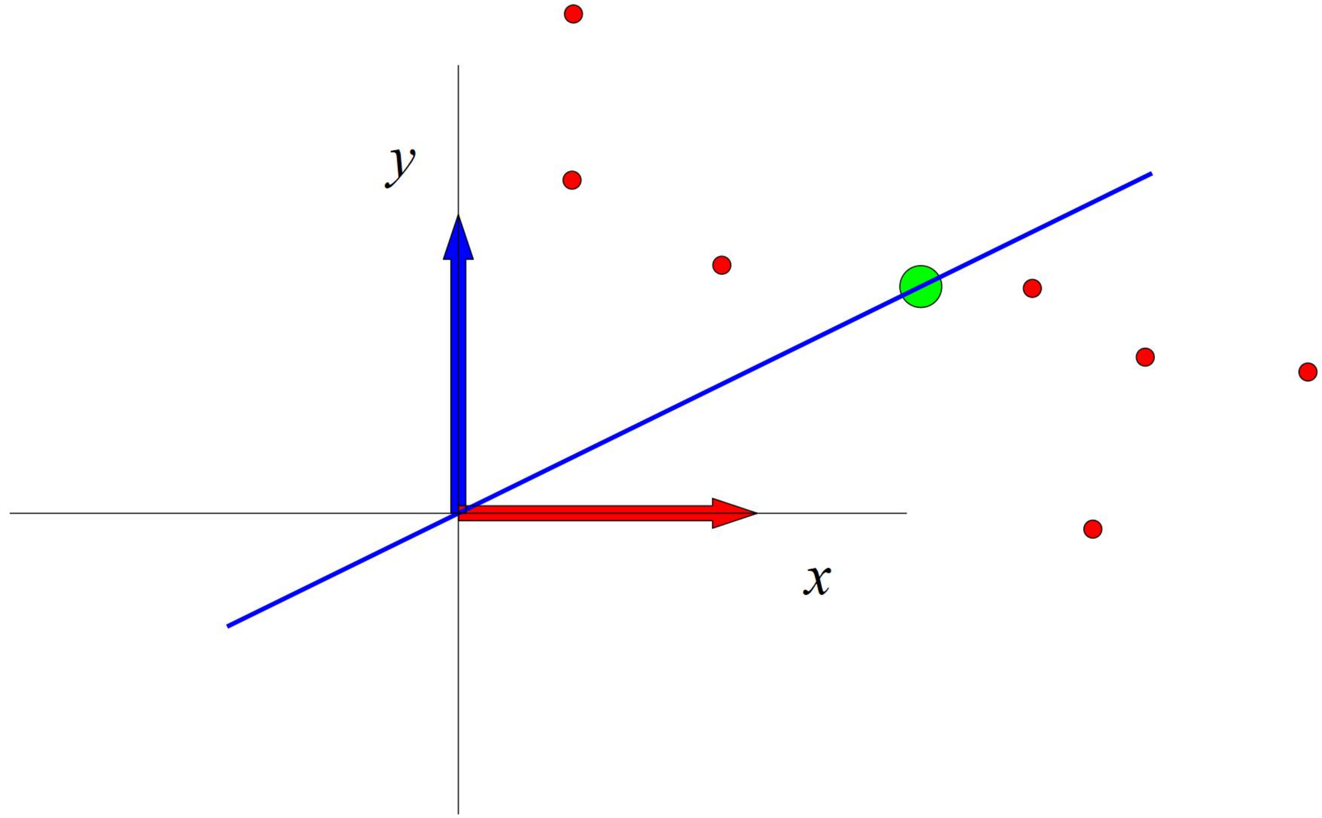
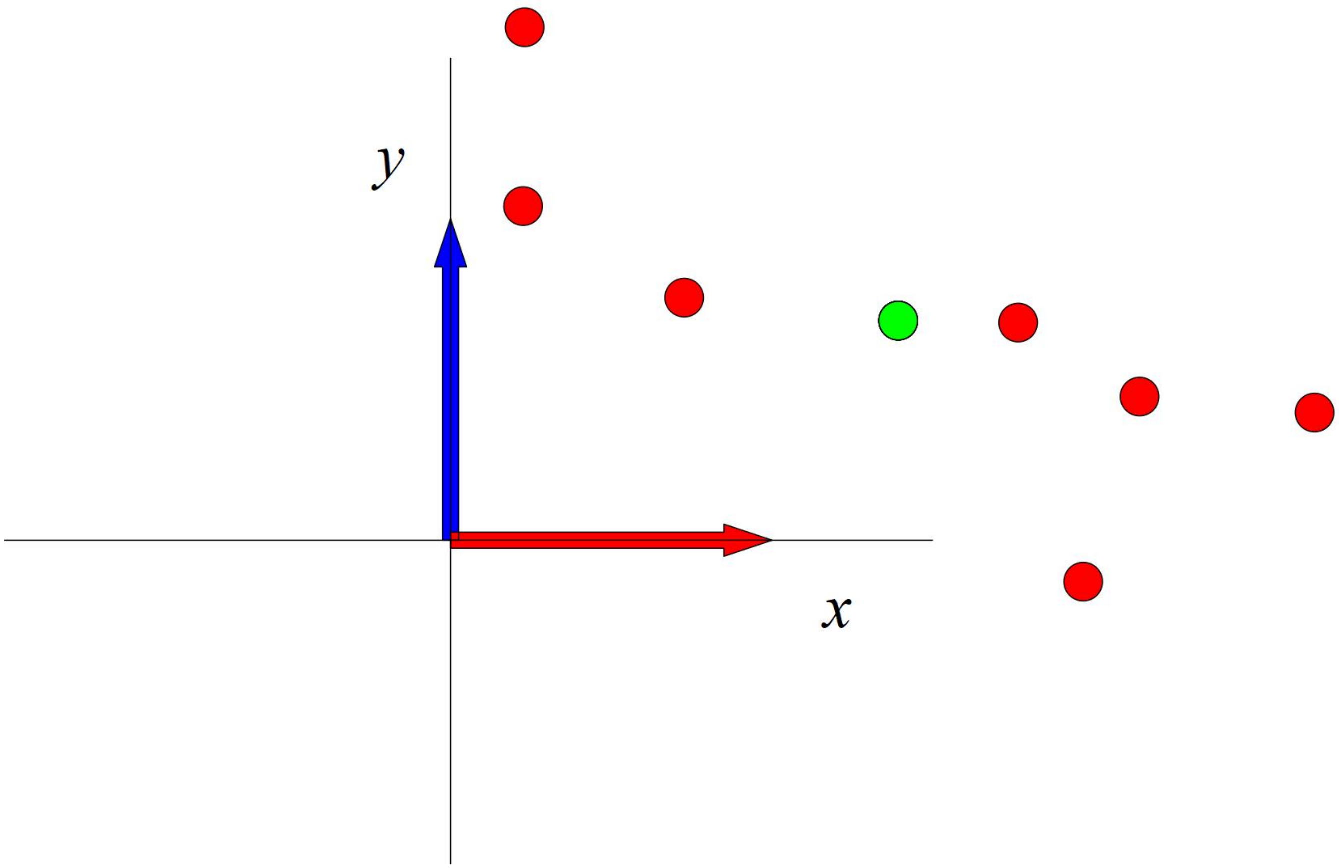
Back to Basics



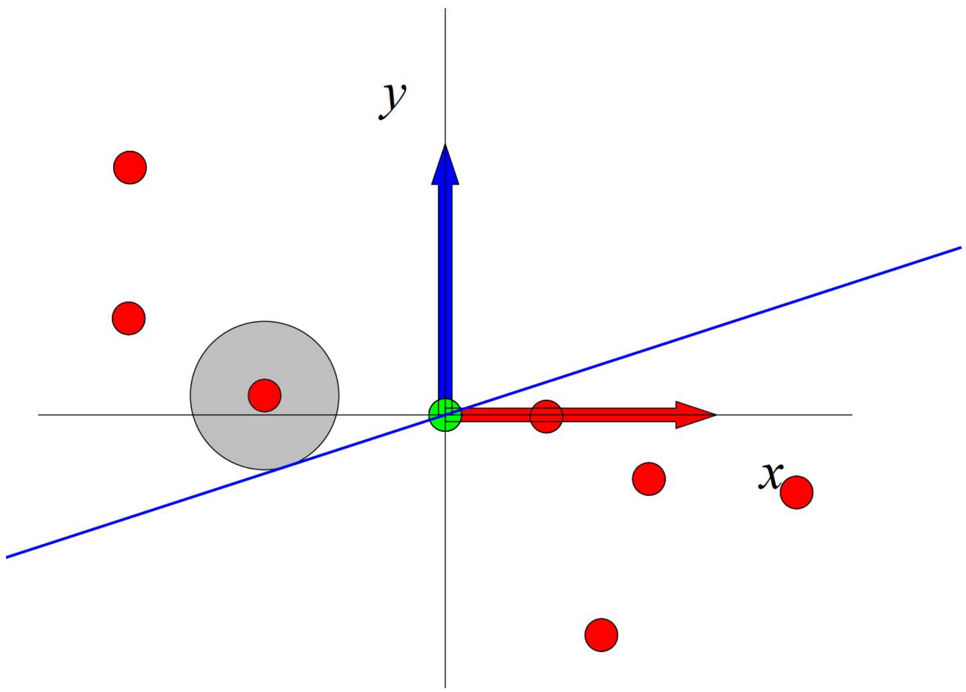
Bedste docking af en ret linje



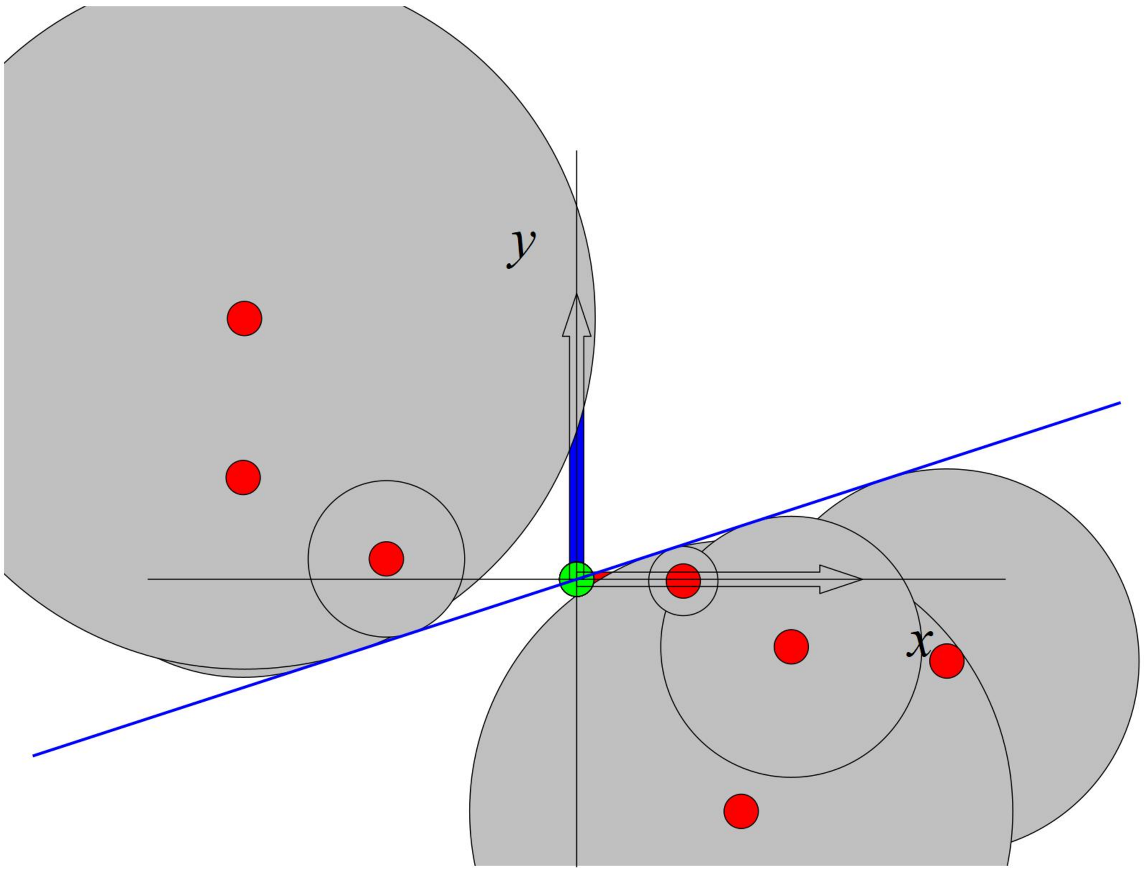
Bedste docking af en ret linje



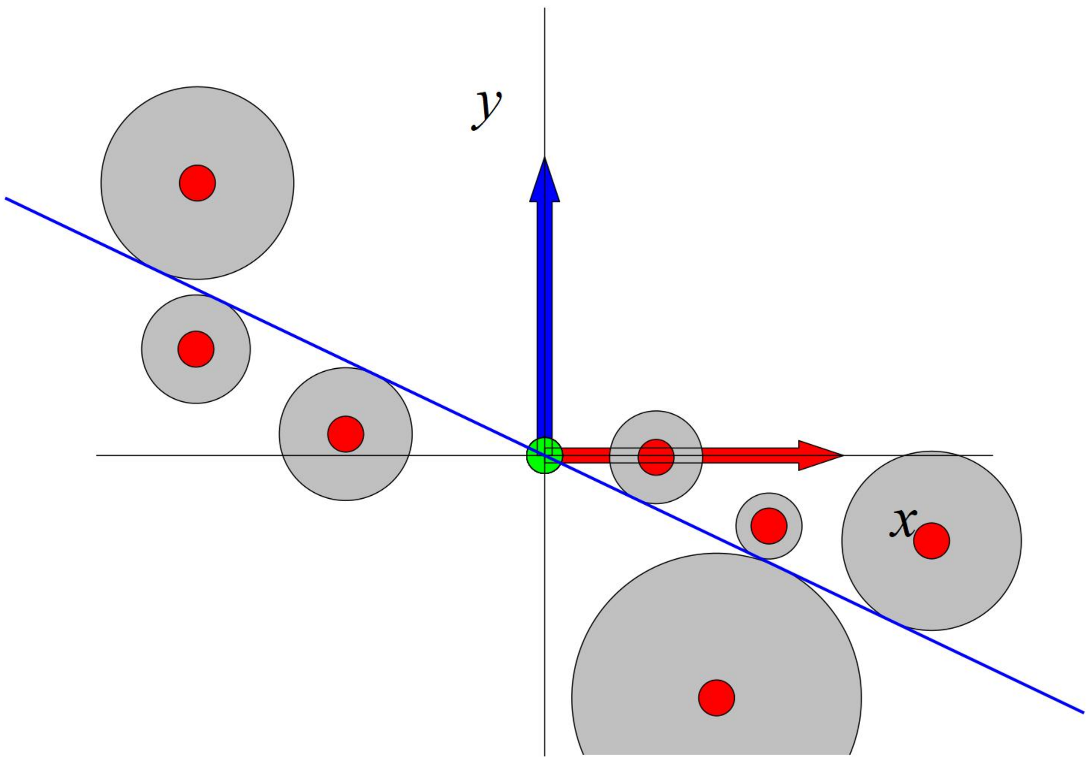
Bedste docking af en ret linje



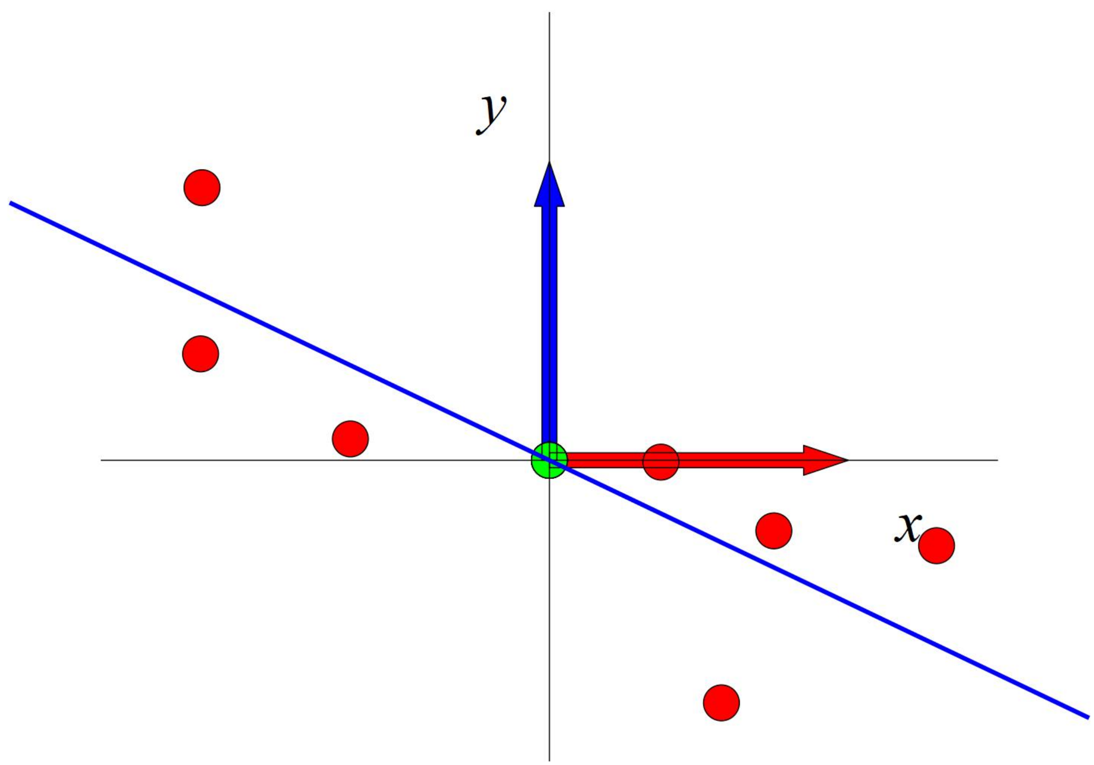
Bedste docking af en ret linje



Bedste docking af en ret linje



Bedste docking af en ret linje



Data-matrix for en plan 7-punktsmængde

$$M = \begin{bmatrix} -0.39 & 0.19 & 0.58 & -1.37 & -0.89 & 0.99 & 0.89 \\ -0.54 & 0.32 & 0.53 & -0.55 & -0.83 & 0.09 & 0.98 \end{bmatrix}$$

Co-varians-matricen for punktmængden

En generel (2×7)-datamatrix M for 7 punkter i planen:

$$M = \begin{bmatrix} x_1 & x_2 & \cdots & x_7 \\ y_1 & y_2 & \cdots & y_7 \end{bmatrix} \quad . \tag{1}$$

Produktet af M med sin egen transponerede matrix $M^\top$ giver følgende (2×2)-matrix (co-varians-matricen for punktmængden):

Co-varians-matricen for punktmængden

$$M \cdot M^\top = \begin{bmatrix} x_1 & x_2 & \cdots & x_7 \\ y_1 & y_2 & \cdots & y_7 \end{bmatrix} \cdot \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ x_7 & y_7 \end{bmatrix} \tag{2}$$

$$= \begin{bmatrix} \sum x_i^2 & \sum x_i \cdot y_i \\ \sum y_i \cdot x_i & \sum y_i^2 \end{bmatrix}$$

Inertimoment-matricer = fejl-matricer

$$S(e) = \sum_{i=1}^{i=n} r^2(p_i, L_e) = \begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot \mathrm{Im} \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \quad , \tag{3}$$

hvor

$$\mathrm{Im} = \begin{bmatrix} \sum y_i^2 & -\sum x_i \cdot y_i \\ -\sum y_i \cdot x_i & \sum x_i^2 \end{bmatrix} \quad . \tag{4}$$

Til sammenligning med:

$$M \cdot M^\top = \begin{bmatrix} \sum x_i^2 & \sum x_i \cdot y_i \\ \sum y_i \cdot x_i & \sum y_i^2 \end{bmatrix} \quad . \tag{5}$$

Inertimoment-matricer = fejl-matricer

Bevis. Fejlen fra et punkt $p = (x, y)$ til linjen L_e igennem $(0, 0)$:

$$\begin{aligned}
S(e) = r^2(p, L_e) &= x^2 + y^2 - (e\cdot(x, y)) \\
&= x^2 + y^2 - (e_1^2 \cdot x^2 + e_2^2 \cdot y^2 + 2e_1 e_2 \cdot xy) \\
&= (1 - e_1^2) \cdot x^2 + (1 - e_2^2) \cdot y^2 - 2e_1 e_2 \cdot xy \\
&= e_2^2 \cdot x^2 + e_1^2 \cdot y^2 - 2e_1 e_2 \cdot xy \\
&= e_1^2 \cdot y^2 - 2e_1 e_2 \cdot xy + e_2^2 \cdot x^2 \\
\\
&= \begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot \begin{bmatrix} y^2 & -xy \\ -yx & x^2 \end{bmatrix} \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}
\end{aligned} \tag{6}$$

□

SVD af (2×7) data-matricen

$$M = U \cdot \Sigma \cdot V^\top \tag{7}$$

$$\begin{aligned}
U &= \begin{bmatrix} | & | \\ u_1 & u_2 \\ | & | \end{bmatrix} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \\
V^\top &= \begin{bmatrix} -- & v_1 & -- \\ -- & v_2 & -- \\ -- & v_3 & -- \\ -- & v_4 & -- \\ -- & v_5 & -- \\ -- & v_6 & -- \\ -- & v_7 & -- \end{bmatrix} \\
\Sigma &= \begin{bmatrix} \sigma_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad .
\end{aligned} \tag{8}$$

Inertimoment-matricer = fejl-matricer

$$S(e) = \sum_{i=1}^{i=n} r^2(p^i, L_e) = \begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot \mathrm{Im} \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \quad , \qquad (9)$$

hvor Im nu kan relateres direkte til dekompositionen af M:

$$\mathrm{Im} = U \cdot \begin{bmatrix} \sigma_2^2 & 0 \\ 0 & \sigma_1^2 \end{bmatrix} \cdot U^\top$$

Inertimoment-matricer = fejl-matricer

Det følger af:

$$
\begin{aligned}
\mathrm{Im} &= \begin{bmatrix} \sum_i y_i^2 & -\sum_i x_i \cdot y_i \\ -\sum_i y_i \cdot x_i & \sum_i x_i^2 \end{bmatrix} \\
&= \mathrm{Spor}\left(M \cdot M^\top\right) \cdot E - M \cdot M^\top \\
&= U \cdot \begin{bmatrix} \sigma_1^2 + \sigma_2^2 & 0 \\ 0 & \sigma_1^2 + \sigma_2^2 \end{bmatrix} \cdot U^\top - U \cdot \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \cdot U^\top \\
&= U \cdot \begin{bmatrix} \sigma_2^2 & 0 \\ 0 & \sigma_1^2 \end{bmatrix} \cdot U^\top \quad ,
\end{aligned}
\tag{10}
$$

Inertimoment-matricer = fejl-matricer

Sætning 1. *Mindste og største inertimoment (og dermed kvadrat fejl) for punktmængden M aflæses som σ^2-værdierne, σ_2^2 og σ_1^2 henholdsvis, og de tilsvarende retninger – de principale retninger – aflæses i U-matricens søjler.*

Inertimoment-matricer = fejl-matricer

Bevis.

$$
\begin{aligned}
S(e) &= \sum_{i=1}^{i=n} r^2(p^i, L_e) \\
&= \begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot \mathsf{Im} \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \\
&= \begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot U \cdot \begin{bmatrix} \sigma_2^2 & 0 \\ 0 & \sigma_1^2 \end{bmatrix} \cdot U^\top \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \\
&= \left(\begin{bmatrix} e_1 & e_2 \end{bmatrix} \cdot U\right) \cdot \begin{bmatrix} \sigma_2^2 & 0 \\ 0 & \sigma_1^2 \end{bmatrix} \cdot \left(U^\top \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}\right) \quad ,
\end{aligned}
\tag{11}
$$

som antager mindste værdi, σ_2^2, for

$$
U^\top \cdot \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad , \tag{12}
$$

sådan at netop retningsvektoren e for linjen med den mindste fejl findes som første søjle vektor i U.

$\square$

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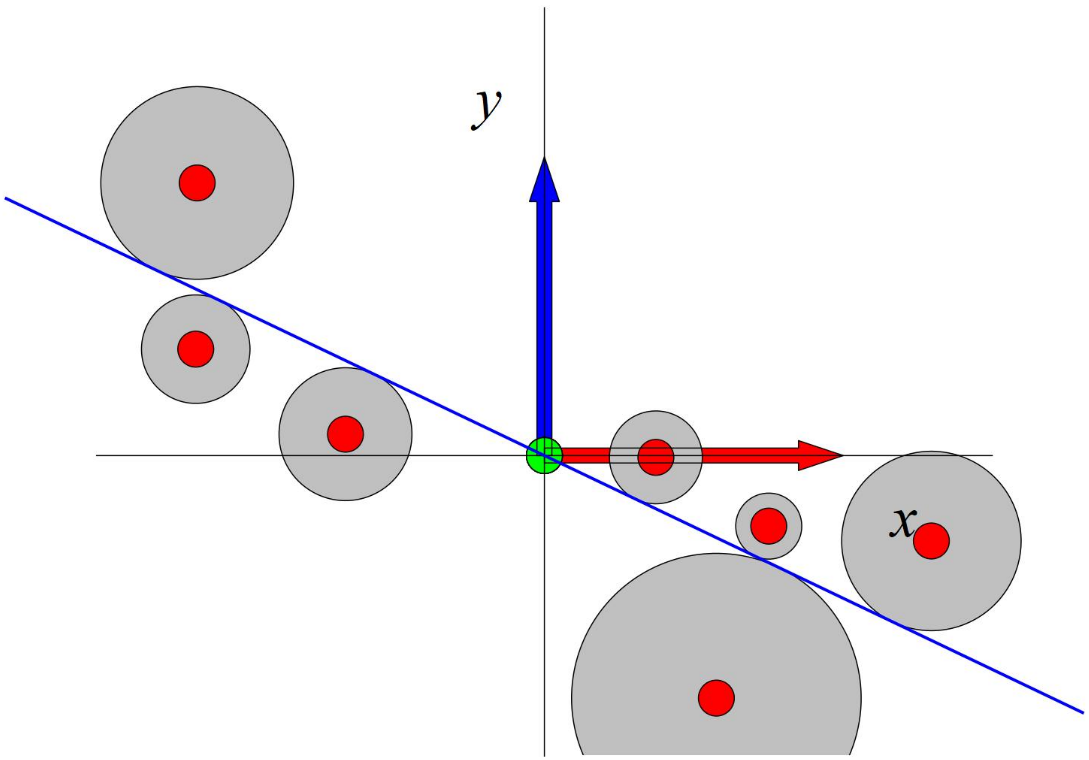

Tak for opmærksomheden!