Beyond Least Squares

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(*joint work with Algo Carè
and Simone Garatti*)

Paul’s day – Eindhoven, 19 April, 2024

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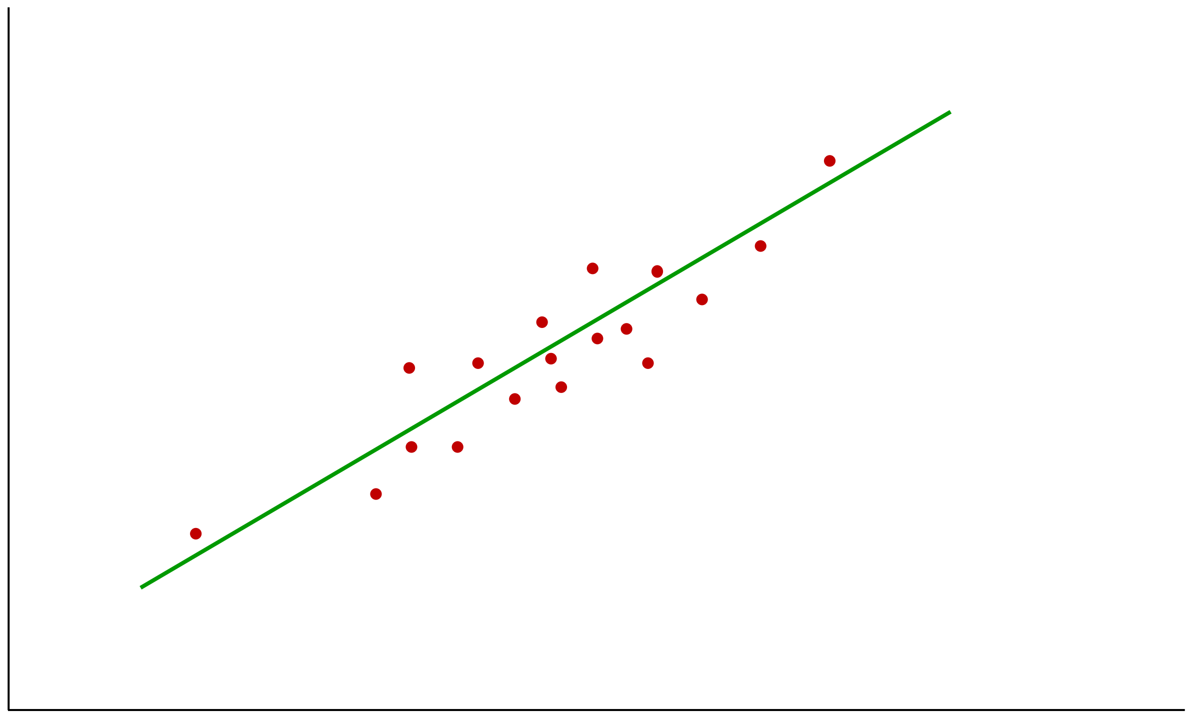
(compromizing is good, … especially true for an Italian man)

Least Squares



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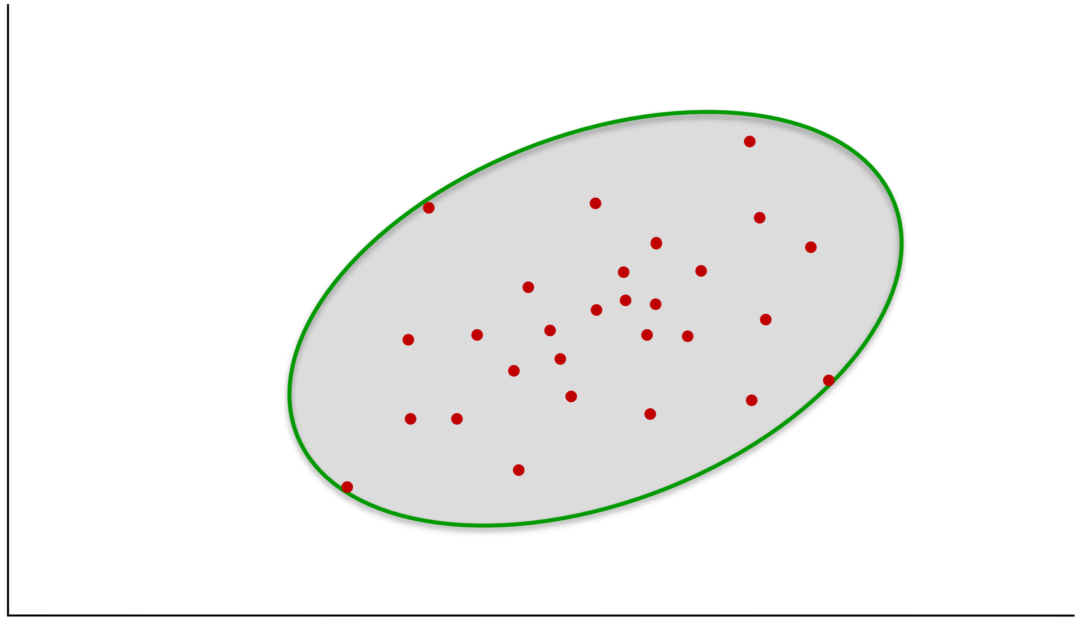
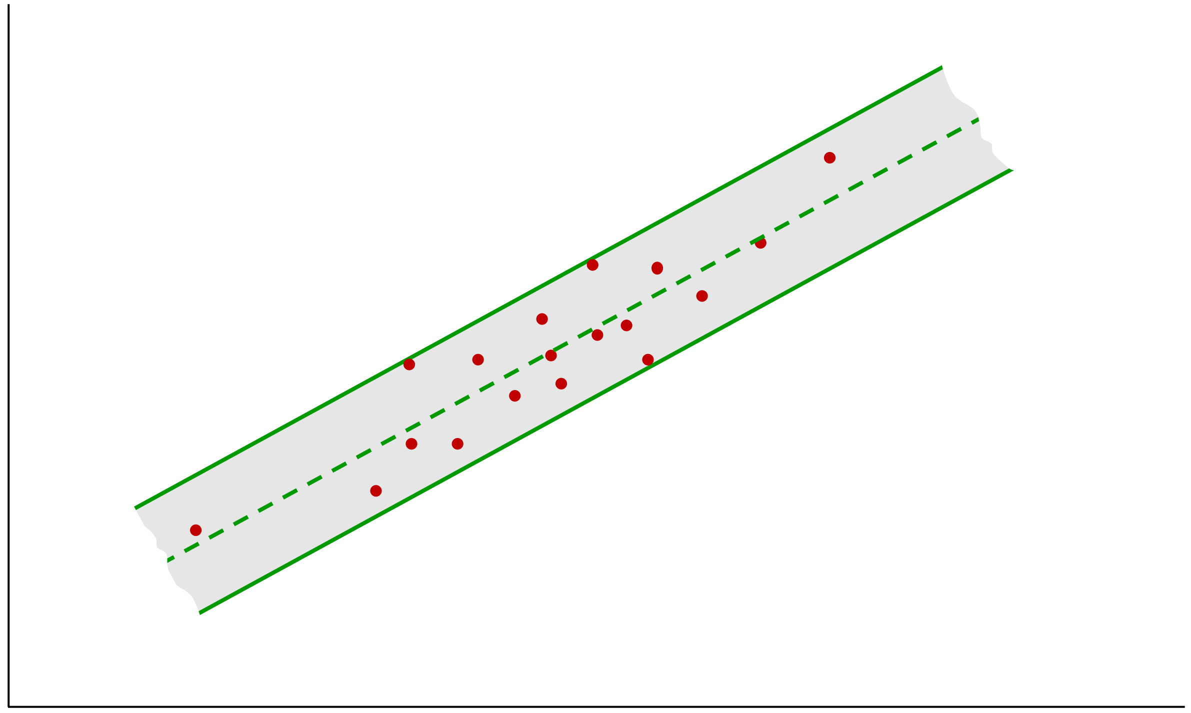


here, the idea is that of “coverage”

… back to example



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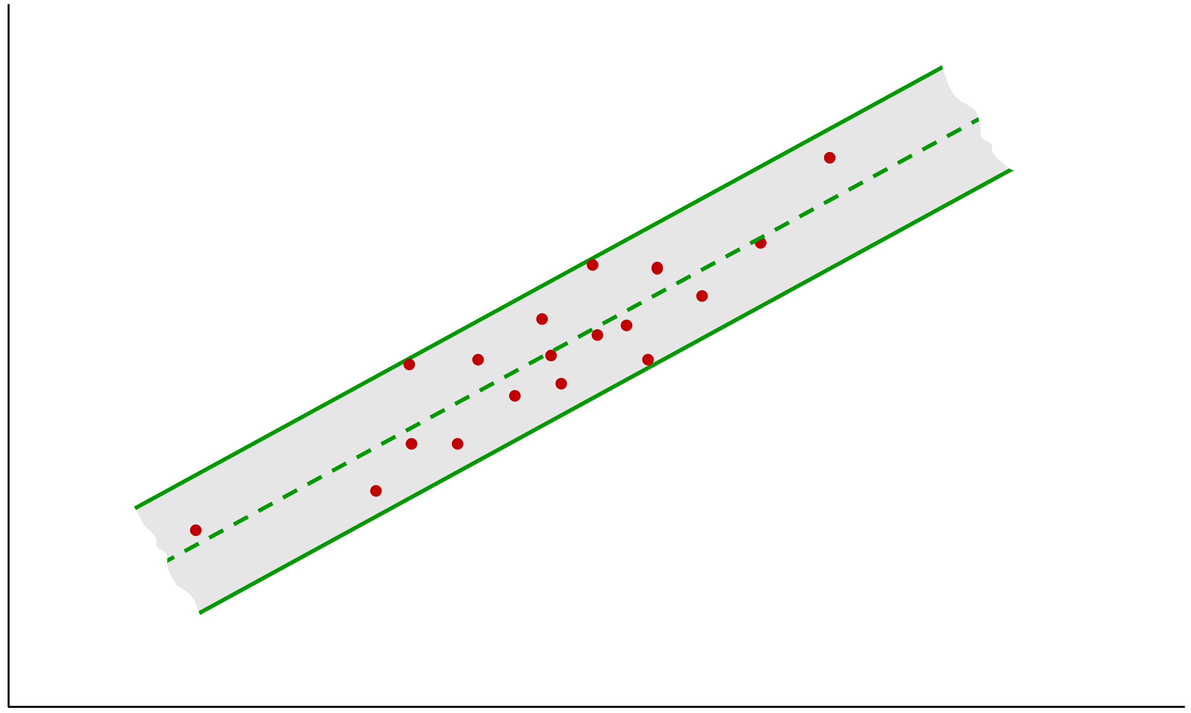
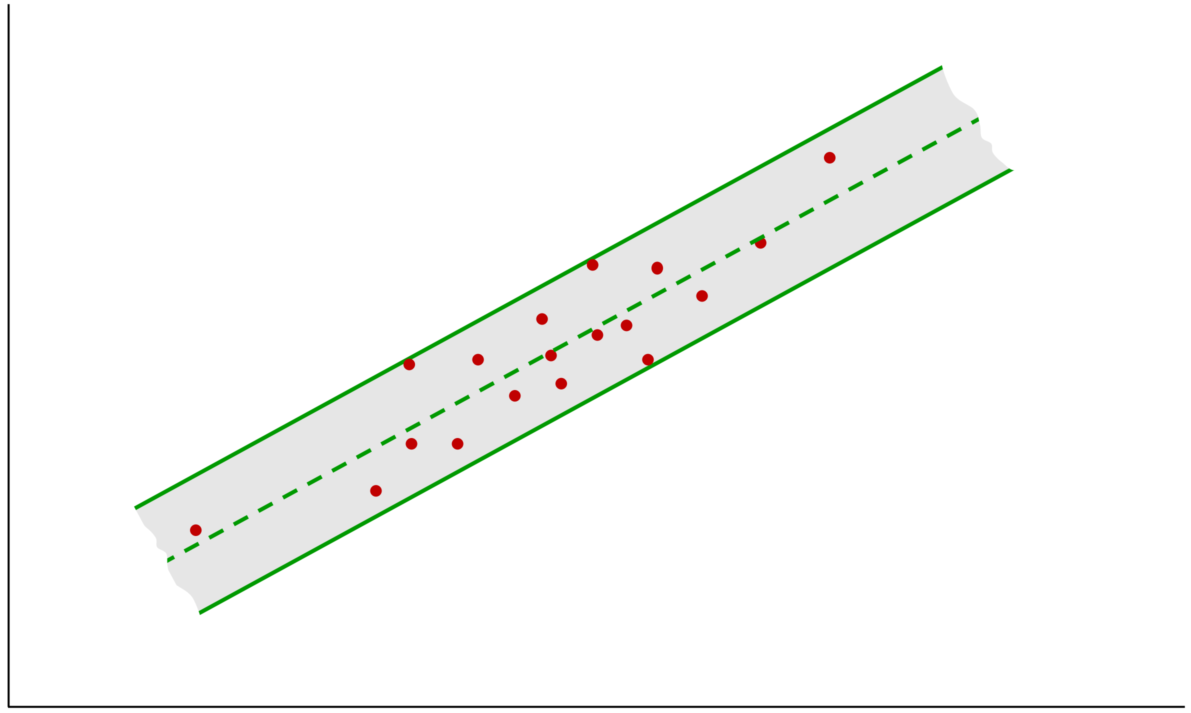


how is this constructed?

minimize size while keeping points inside

… back to example



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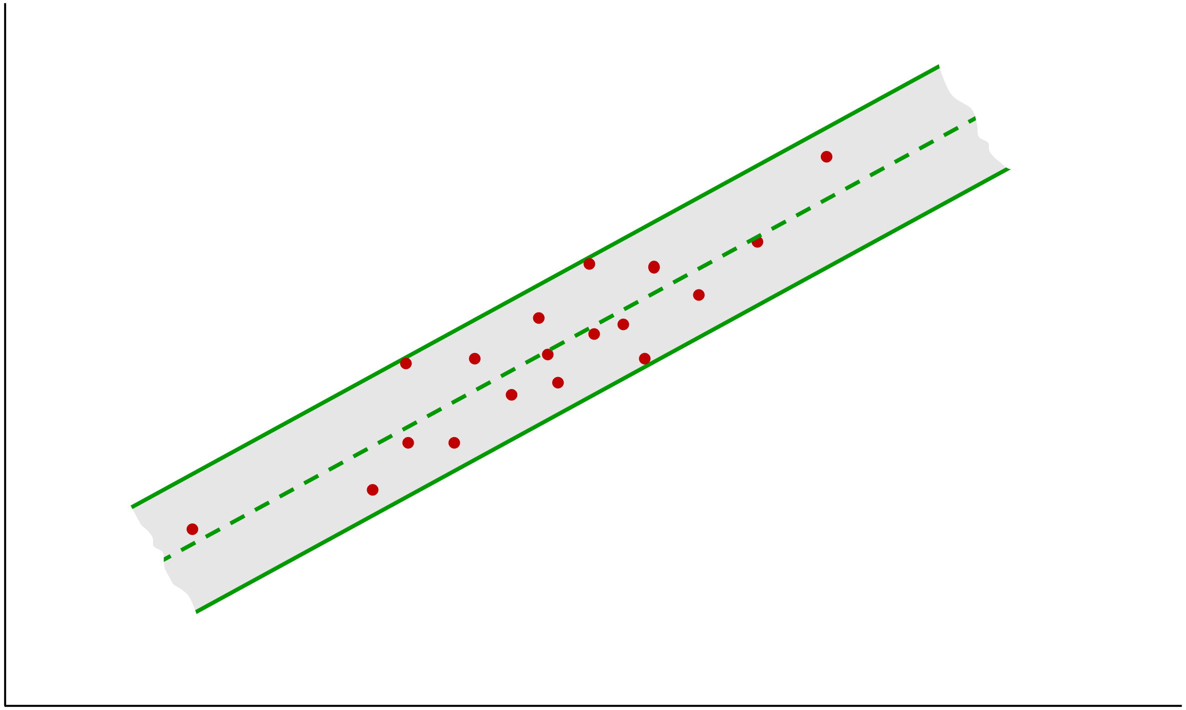
minimize size while keeping points inside
(inherently different from enlarging from LS estimate)

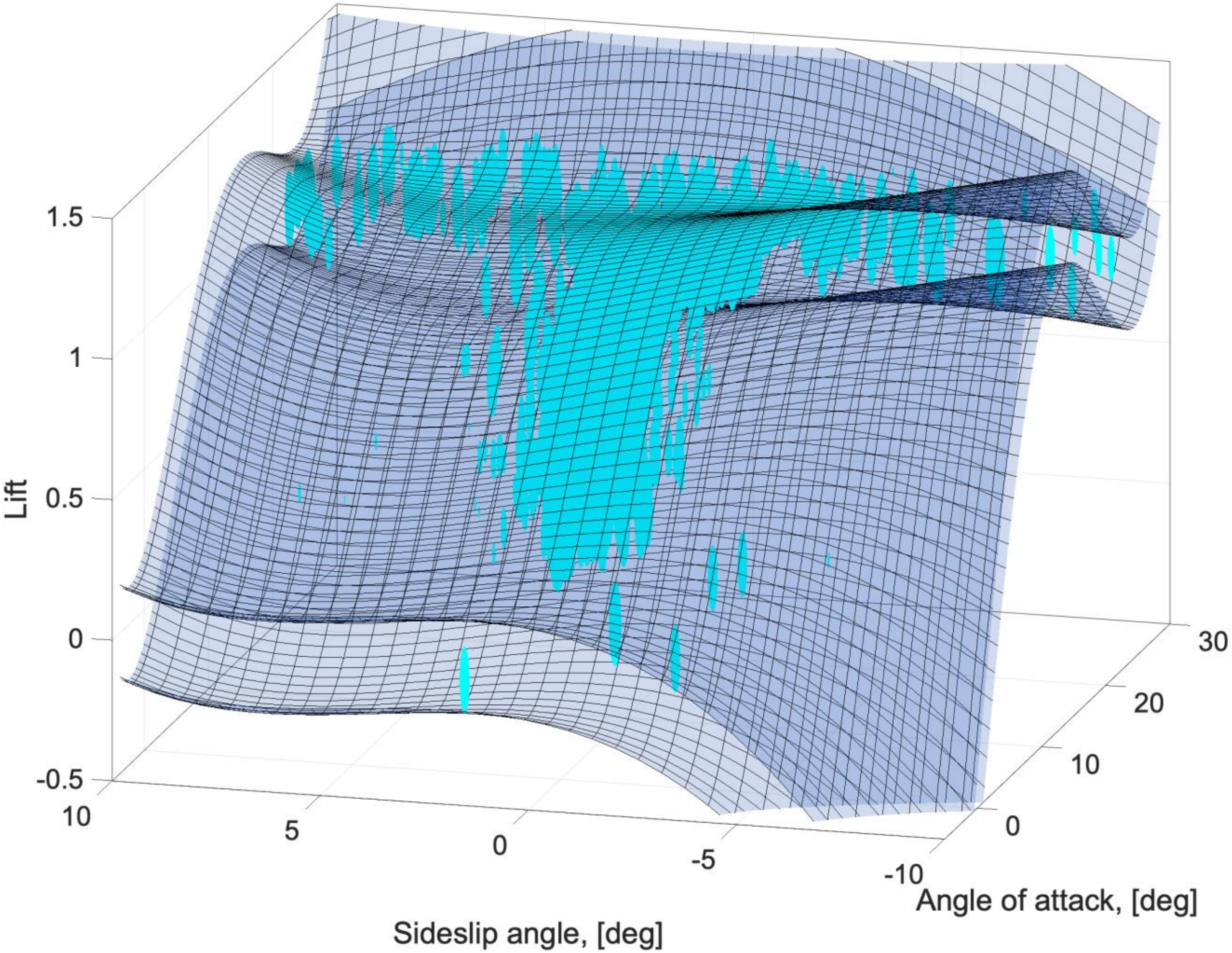
… back to example



in formulas:

$$\min_{\theta} \sum_{i=1}^{N} (y_i - f_\theta(u_i))^2 \quad \Longrightarrow \quad \min_{\theta} \max_{i=1,\ldots,N} |y_i - f_\theta(u_i)|$$

another example



→ *min-max modelling was introduced by Leonhard Euler some half a century before least squares*

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$$\min_{\theta} \max_{i=1,\ldots,N} |y_i - f_\theta(u_i)|$$

$$\Downarrow$$

$$\min_{\theta,\gamma} \gamma$$

$$\text{subject to: } |y_i - f_\theta(u_i)| \leq \gamma$$

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⇓

$$\min_{\theta,\gamma} \gamma$$

$$\text{subject to: } |y_i - f_\theta(u_i)| \le \gamma$$

⇒

$$\min_{\theta,\gamma,\xi_i \ge 0} \gamma + \rho \sum_{i=1}^{N} \xi_i$$

$$\text{subject to: } |y_i - f_\theta(u_i)| - \gamma \le \xi_i$$

relaxation

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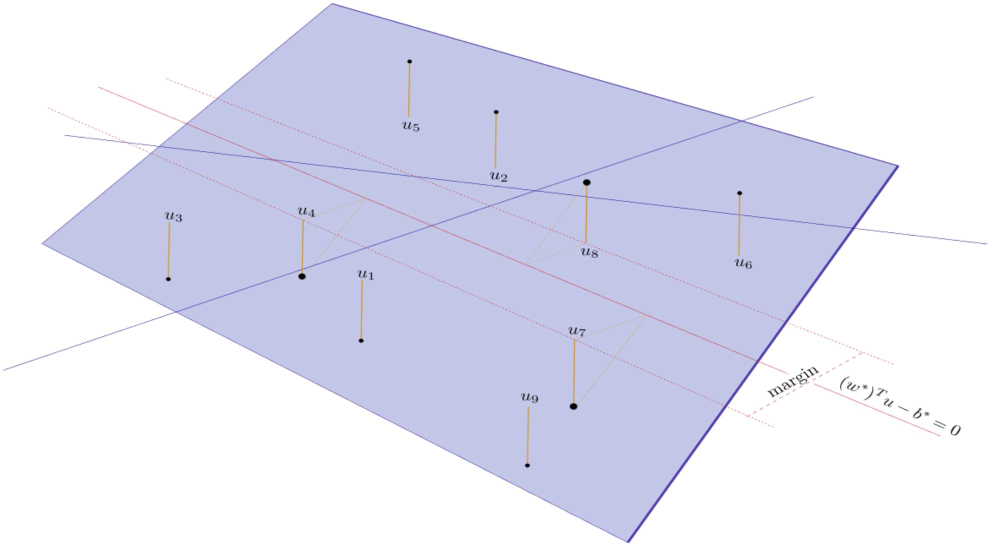
for example, SVM:

$$\min_{w \in \mathbb{R}^d, b \in \mathbb{R}, \xi_i \geq 0} \|w\|^2 + \rho \sum_{i=1}^{N} \xi_i$$

$$\text{subject to: } 1 - y_i(\langle w, u_i \rangle - b) \leq \xi_i$$



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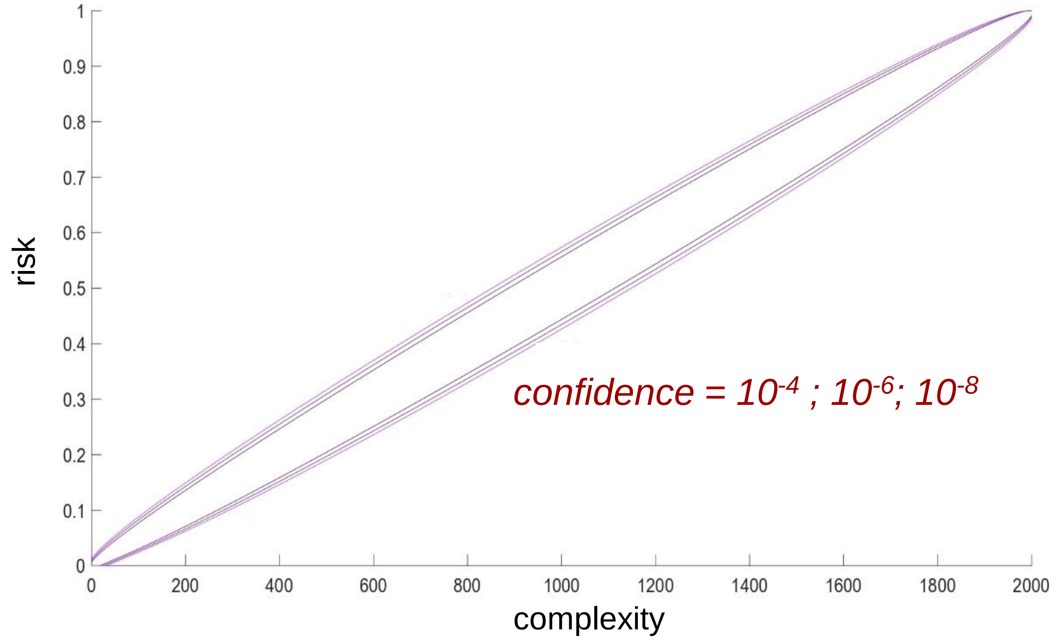

confidence = 10^{-4} ; 10^{-6}; 10^{-8}

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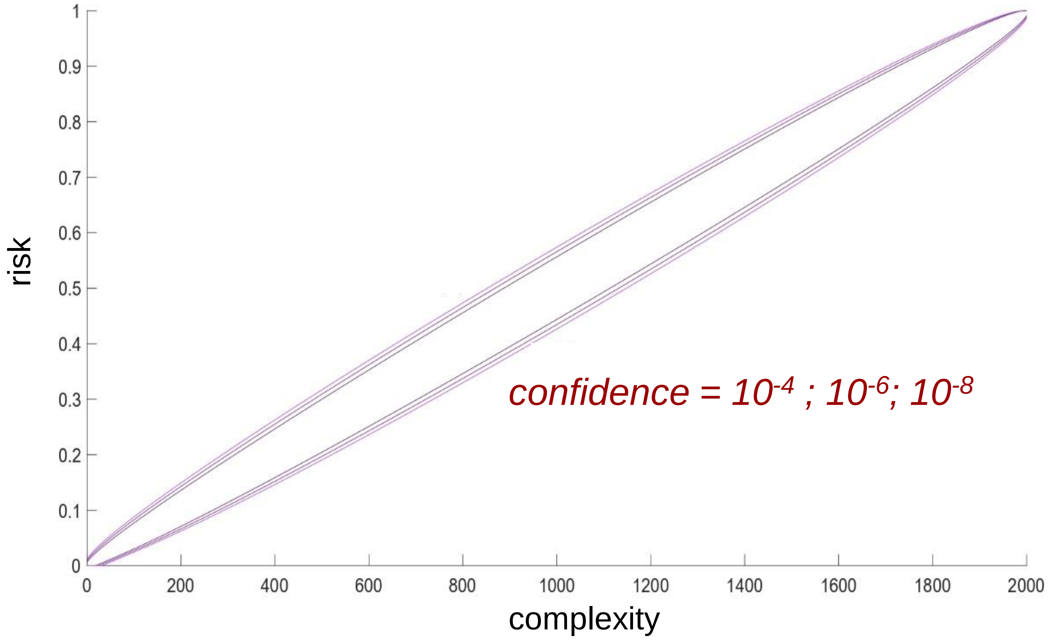

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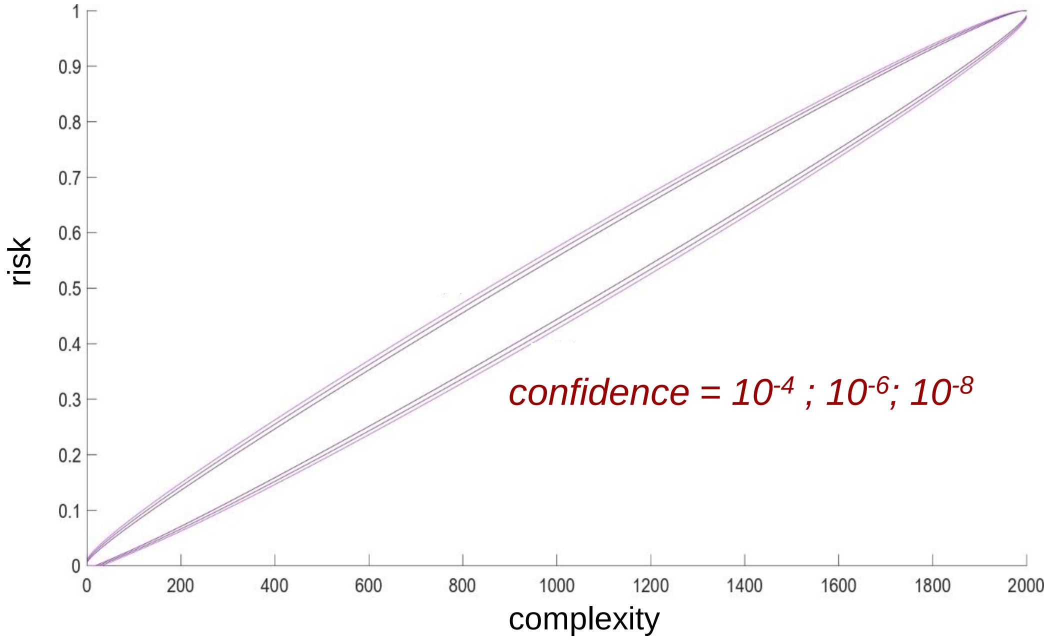

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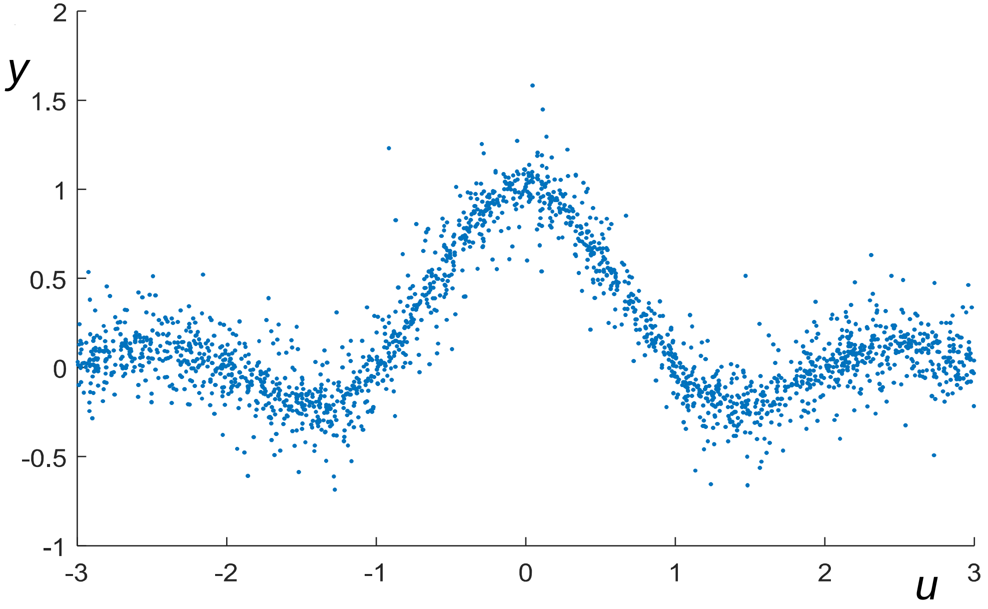
→ *develop trust in the model*

→ *tune hyper-parameters*

Example: SVR

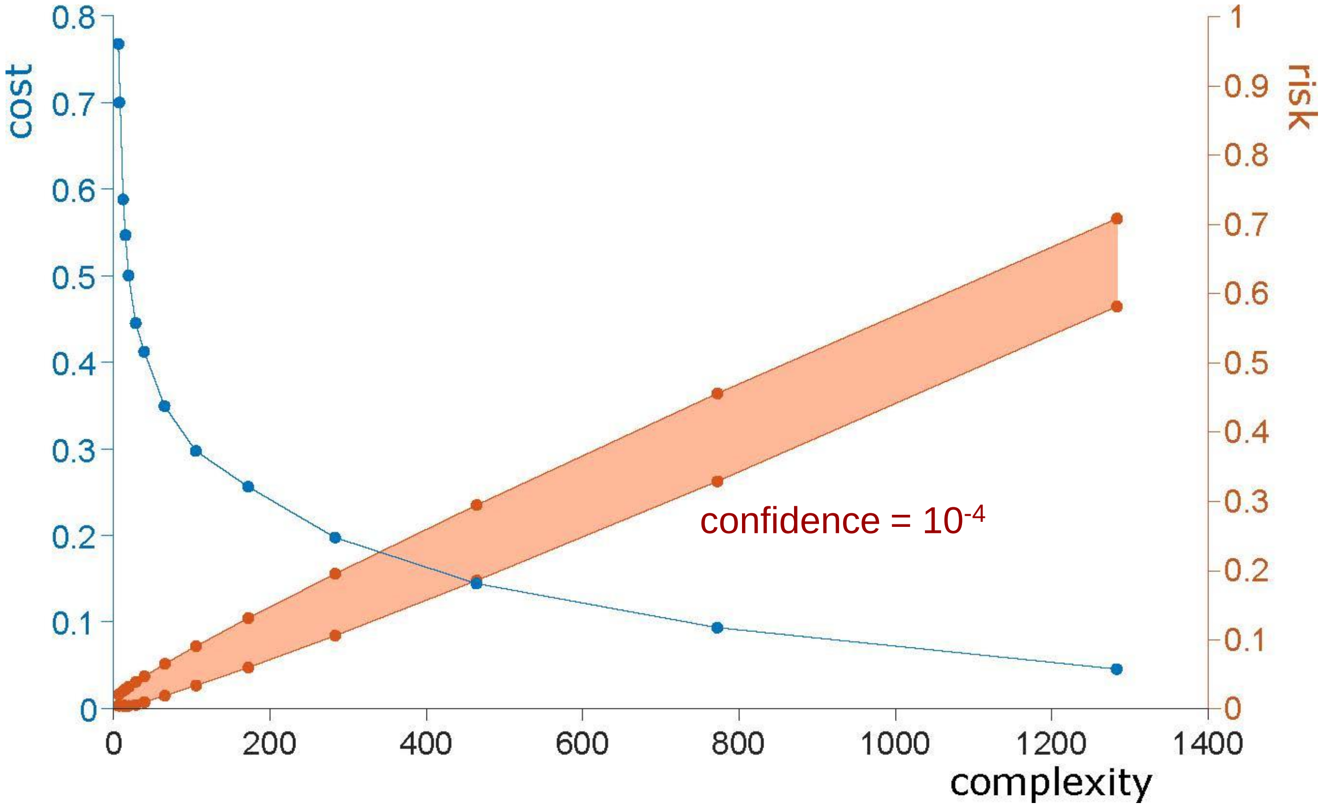


$$\min_{w,\gamma,b,\xi_i\geq 0} (\gamma + 0.01\|w\|^2) + \rho \sum_{i=1}^{N} \xi_i$$

subject to: $|y_i - \langle w, \phi_i \rangle - b| - \gamma \leq \xi_i, \quad i = 1, \ldots, 2000$

$\langle \phi_i, \phi_j \rangle = \exp(-(u_i - u_j))^2$ (Gaussian kernel)

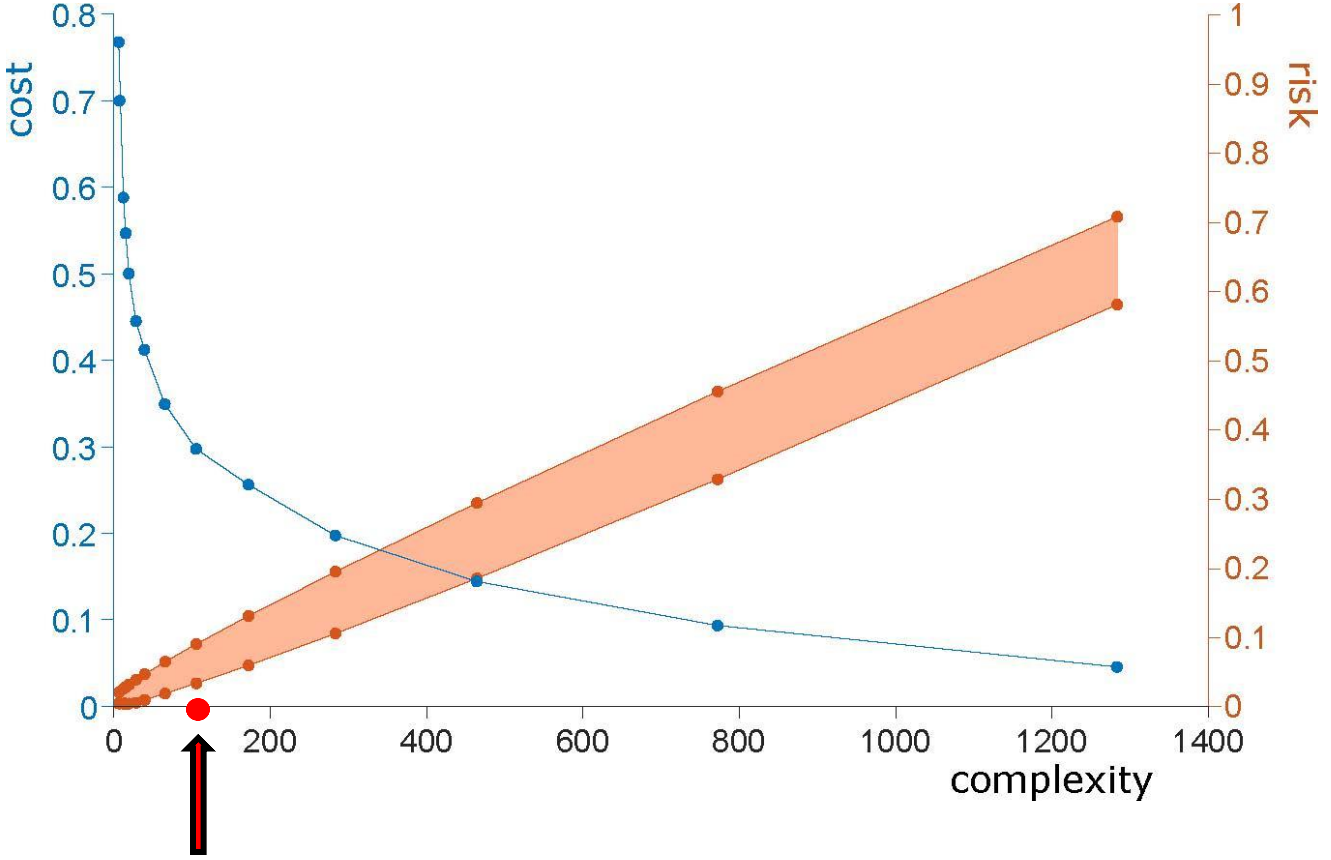
Example: SVR



confidence = 10^{-4}

$$\rho = \left(\frac{3}{5}\right)^{\ell}, \quad \ell = 0, \ldots, 14$$

Example: SVR



$\rho = (3/5)^9$

$\text{risk} \in [0.032, 0.08] \qquad \gamma^* = 0.3$

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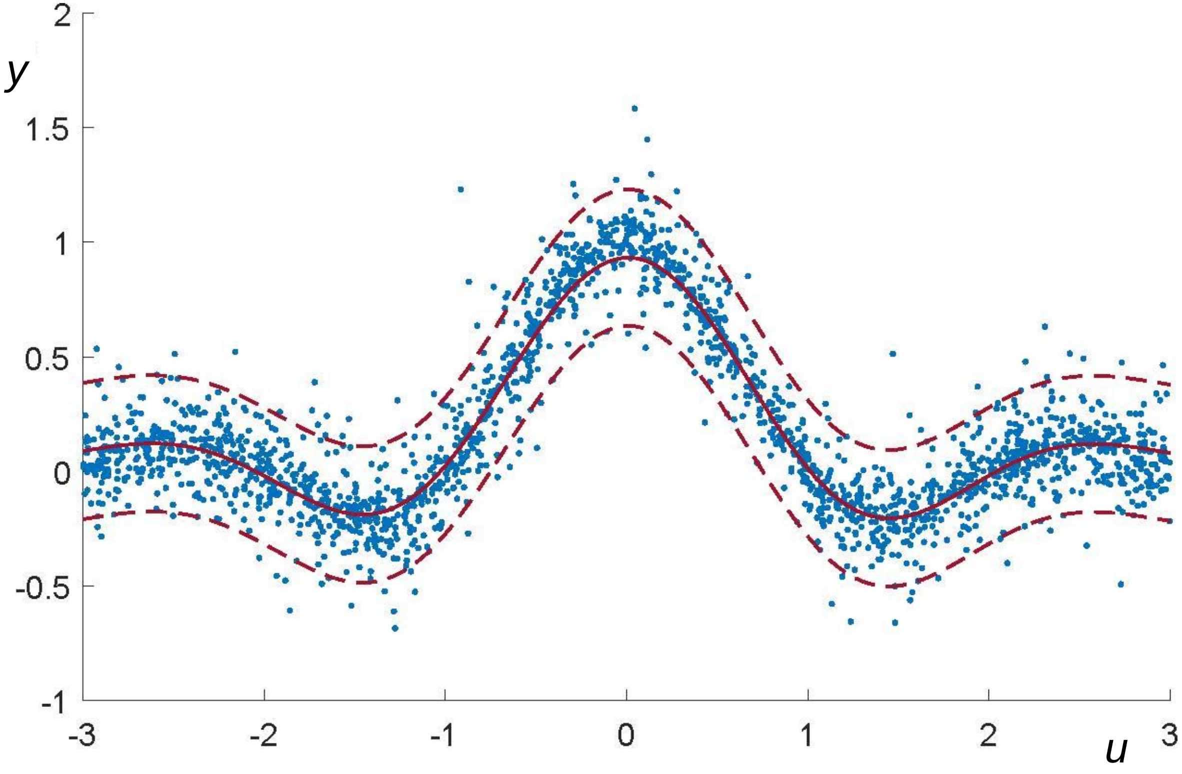

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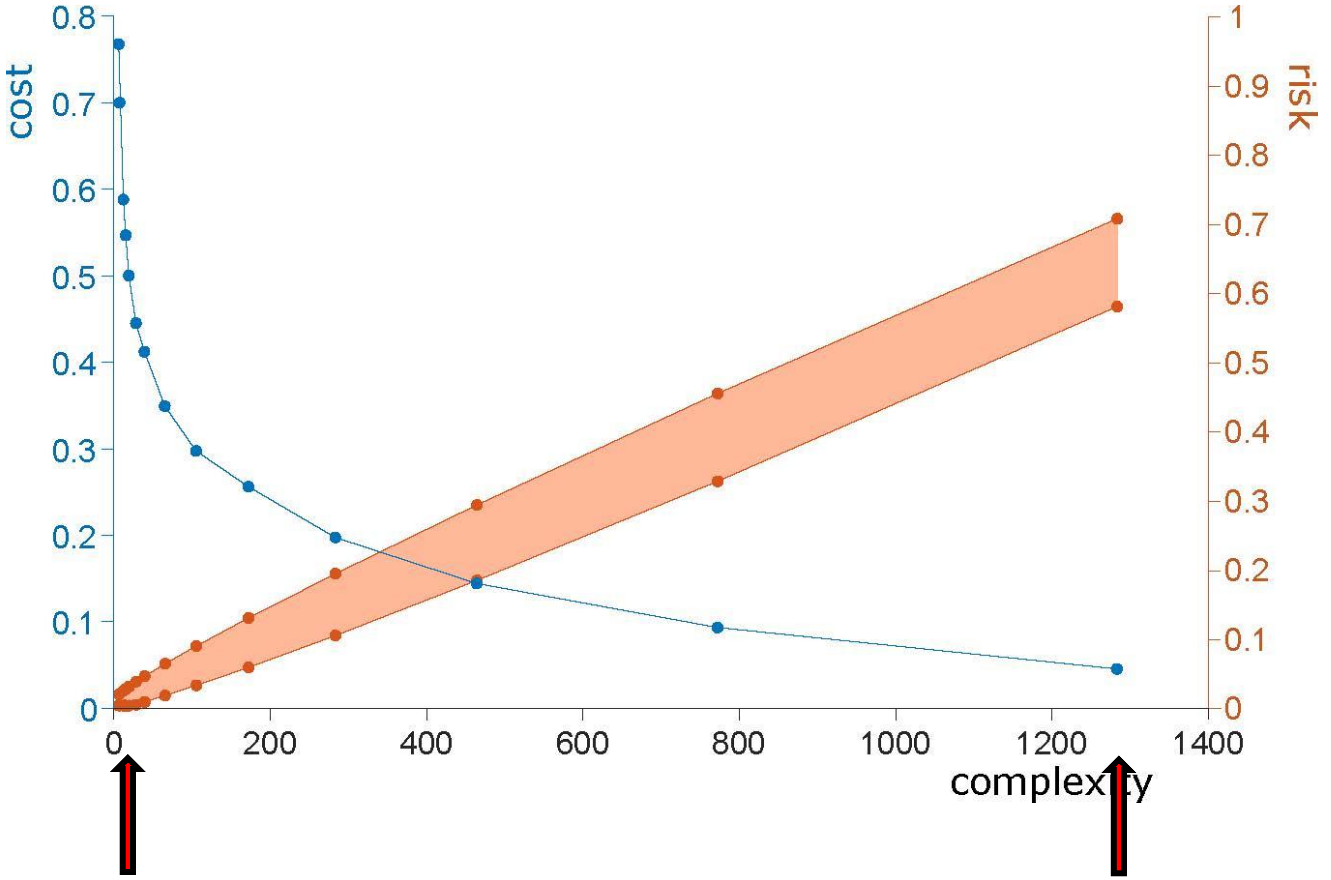

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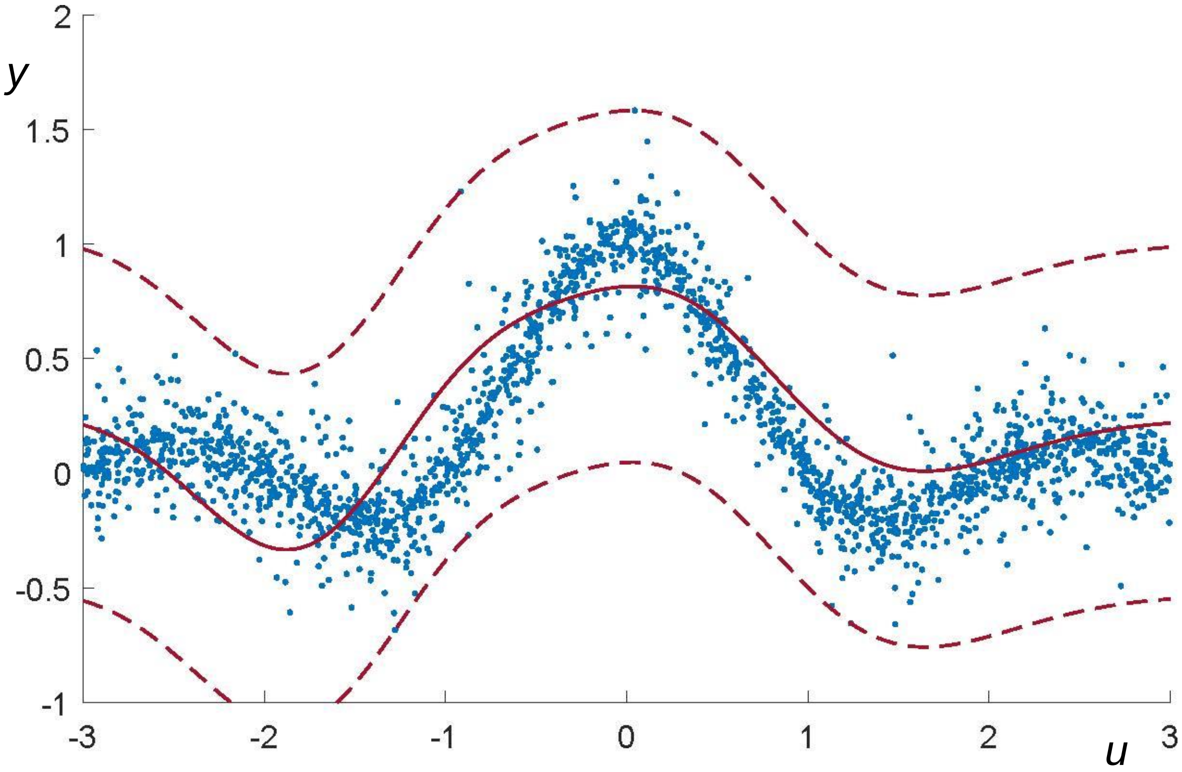

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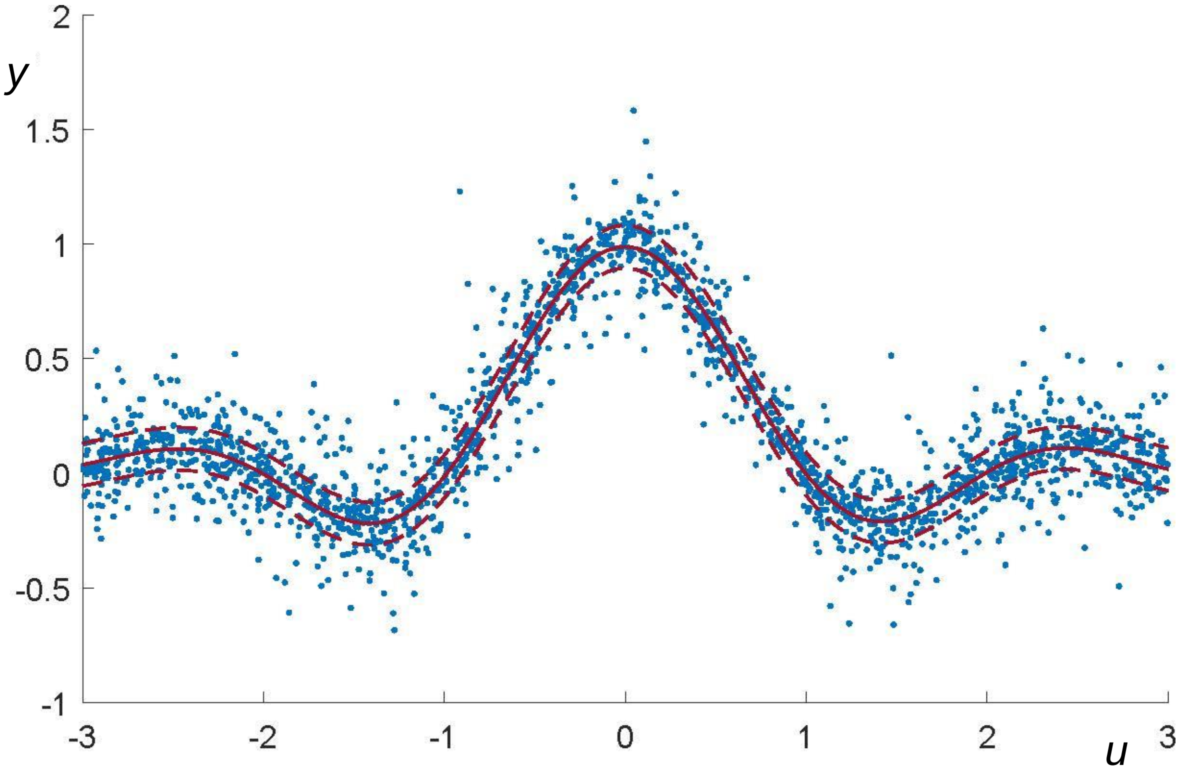

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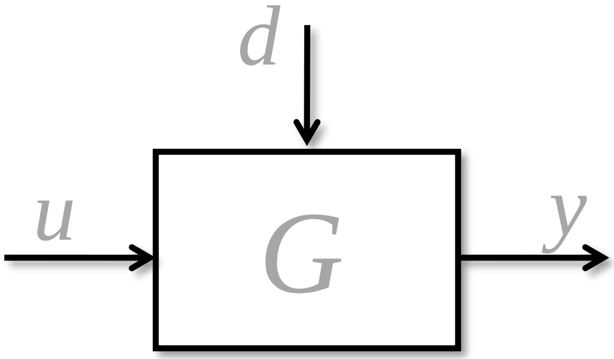

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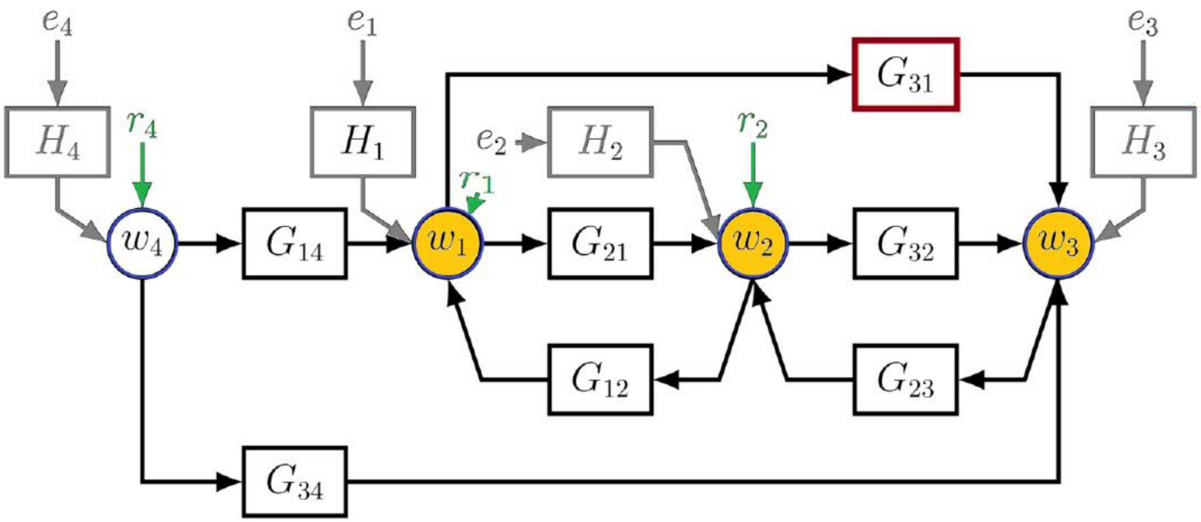

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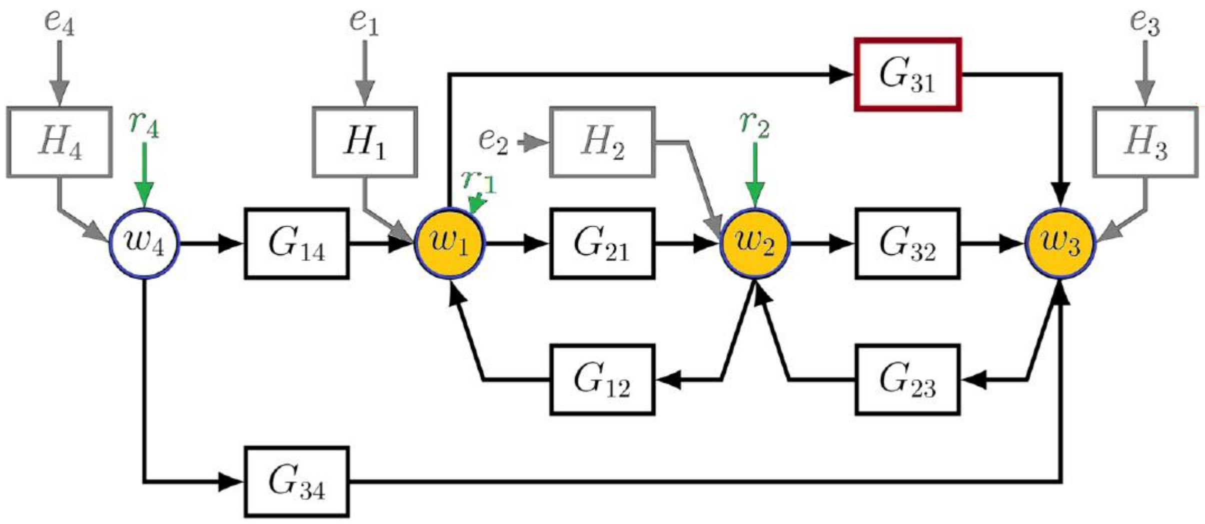

something one of us knows very well!

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Ad maiora, Paul!