Augmented Experiments in Material Engineering Using Machine Learning

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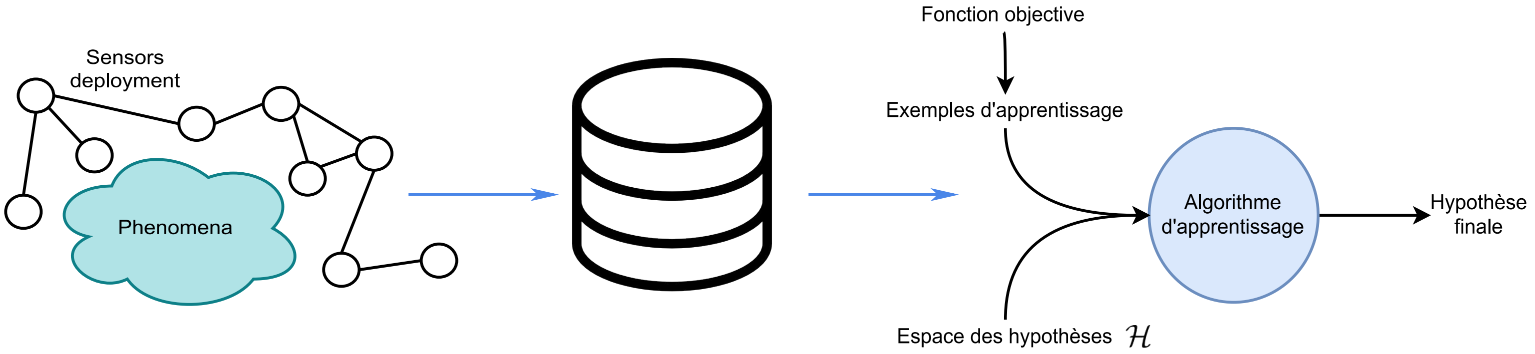
@PFIA'21

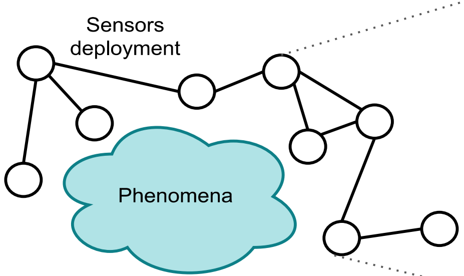
Contexte et motivations

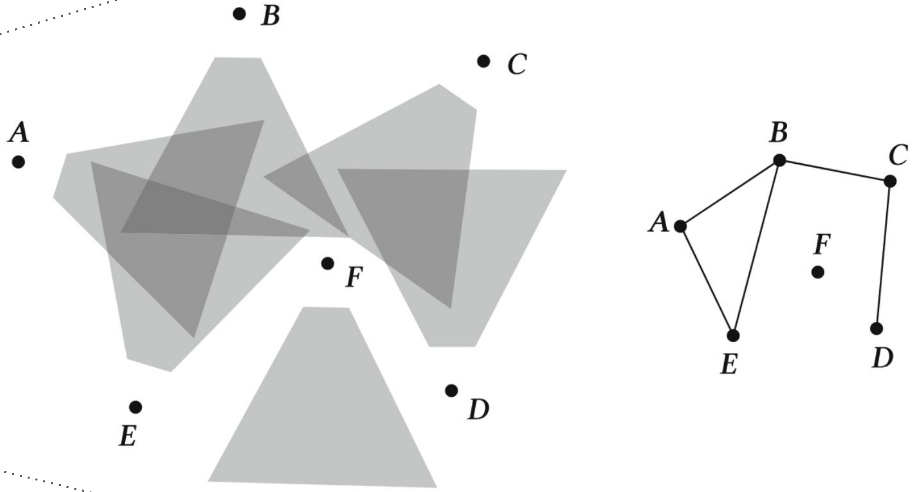
Apprentissage dans l’Internet des objets



Spécificités des déploiements

Topologies des déploiements



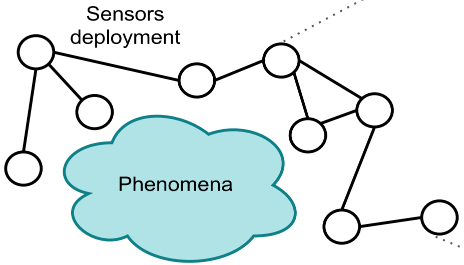


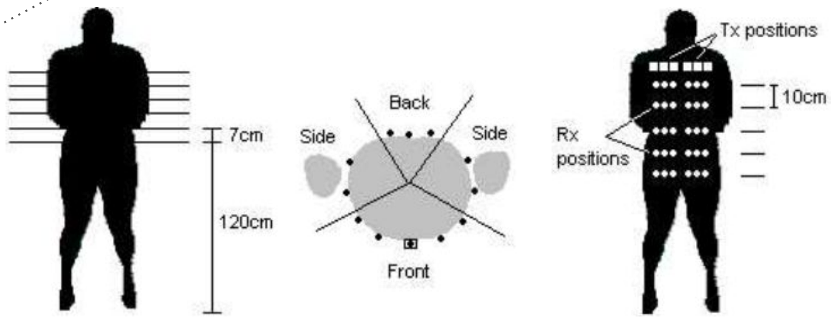
- Plusieurs perspectives (ou vues) : redondantes, complémentaires, contradictoires, etc.;

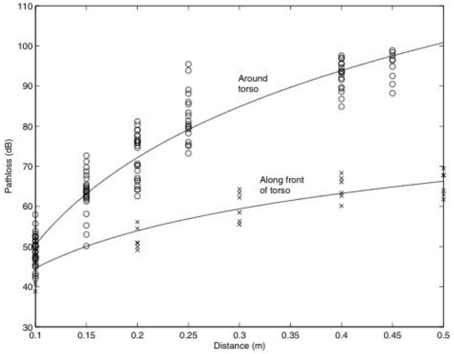
Mavrinac, Aaron, and Xiang Chen. "Modeling coverage in camera networks: A survey." *International journal of computer vision* 2013.

Spécificités des déploiements

Transmissions: Path loss; Shadowing





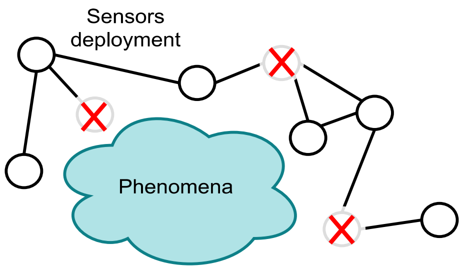


Les transmissions ne s’effectuent que lorsque les conditions favorables sont disponibles (ex. Channel Coherence Time).

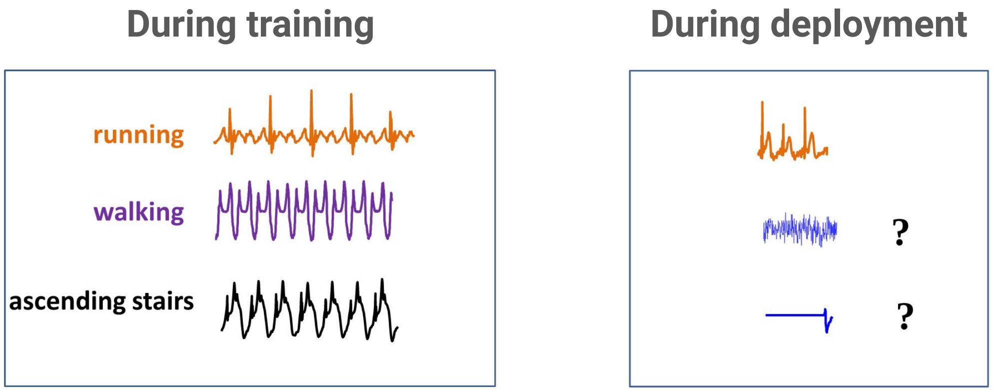
Fort, Andrew, et al. "Characterization of the ultra wideband body area propagation channel." *IEEE International Conference on Ultra-Wideband*. 2005

Apprendre sous des hypothèses plus réalistes

Vues manquantes : accès à une donnée partielle, segment incomplet, etc.

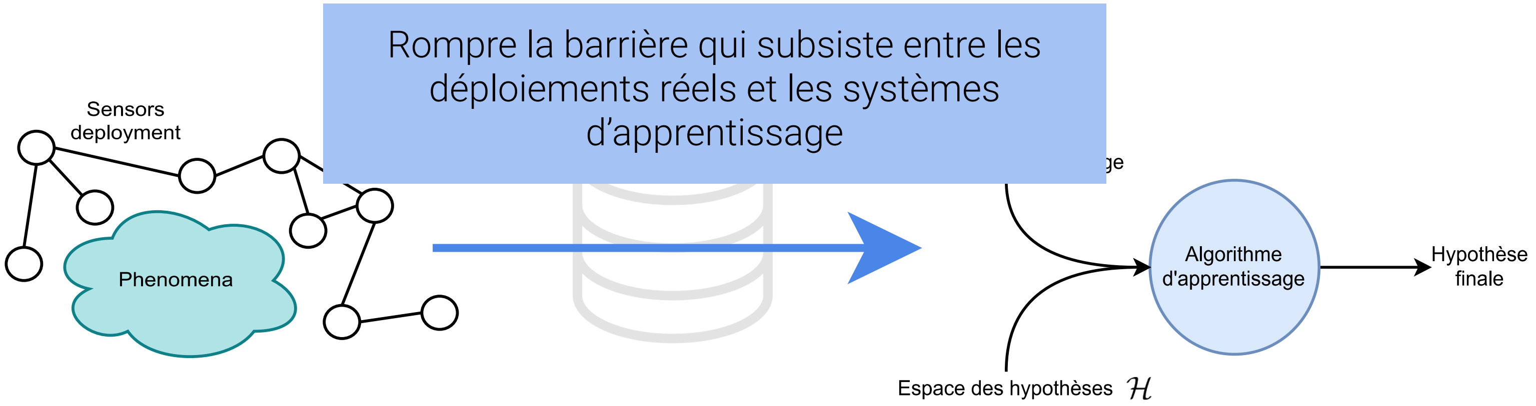


(Unrealistic) Assumption: every item to be classified belongs to exactly one of the well-defined classes



Hu, Bing, Yanping Chen, and Eamonn Keogh. "Time series classification under more realistic assumptions." Proceedings of the 2013 SIAM International Conference on Data Mining. Society for Industrial and Applied Mathematics, 2013.

Apprentissage dans l’Internet des objets



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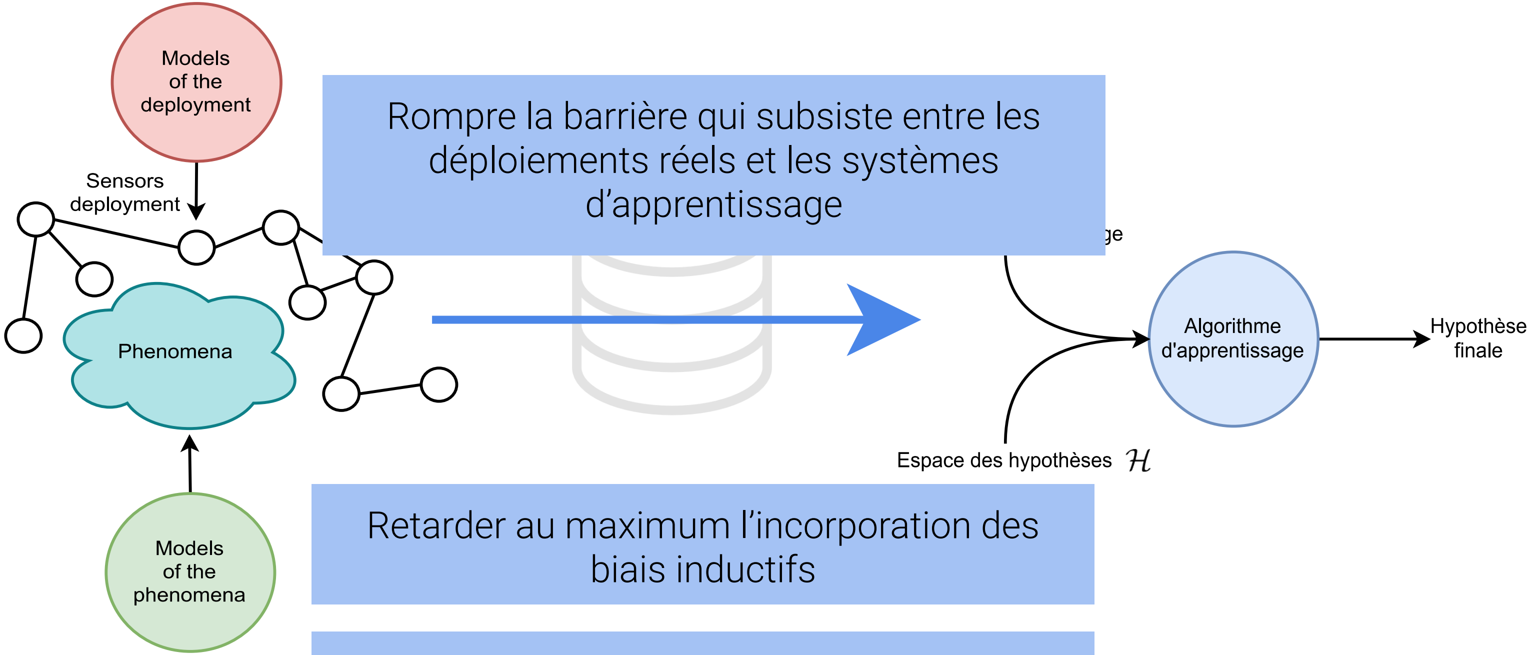


Rompre la barrière qui subsiste entre les déploiements réels et les systèmes d'apprentissage

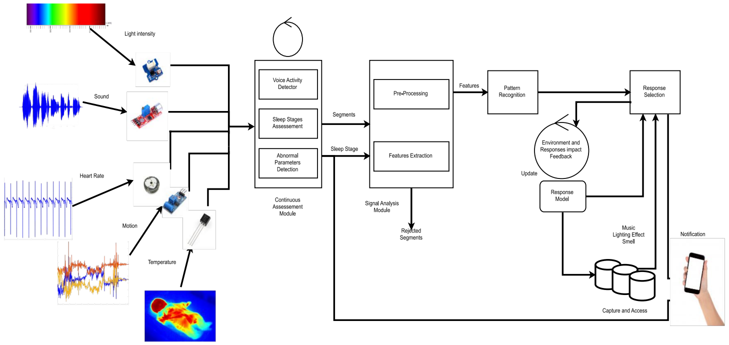
Retarder au maximum l'incorporation des biais inductifs

Apprendre à partir d'exemples et de modèles du domaine

Applications Explorées

Applications Explorées

- Reconnaissance des situations d’inconfort chez les nourrissons ;
- Reconnaissance d’activités humaines ;
- Suivi du phénomène vibratoire des turbocompresseurs ;
- Synthèse de nouveaux matériaux en industrie



A Osmani, M Hamidi, A Chibani. In: *AAAI Fall Symposium Series* 2017

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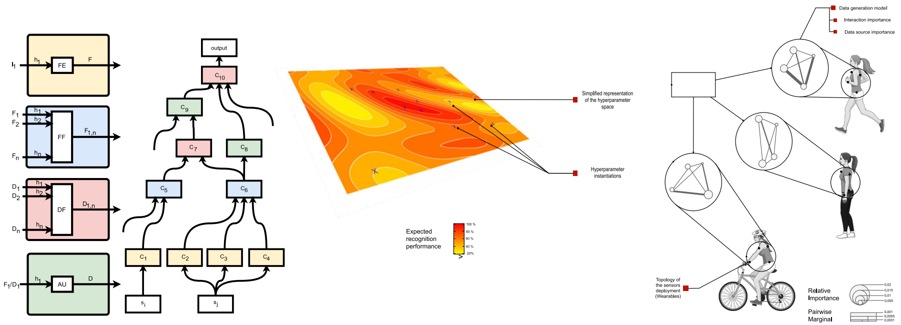

Hamidi, Massinissa and Osmani, Aomar. *Proceedings of the ECML-PKDD* 2020

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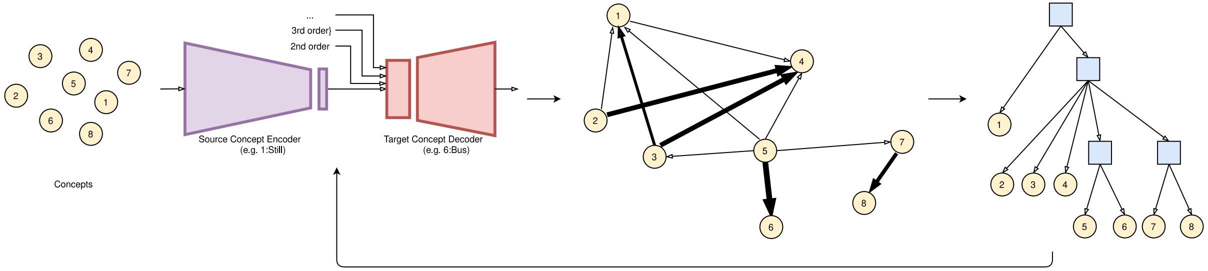

Osmani, Aomar and Hamidi, Massinissa and Alizadeh, Pegah. *Proceedings of the PAKDD* 2021

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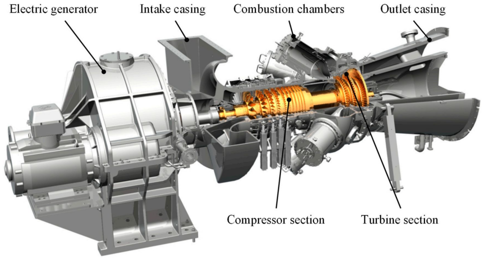
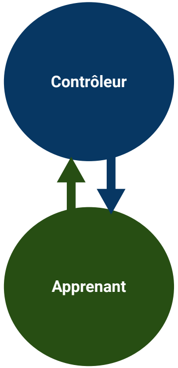


Typical gas turbine construction



Osmani, Aomar and Hamidi, Massinissa and Bouhouche, Salah. *Proceedings of the international joint conference on artificial intelligence* 2019

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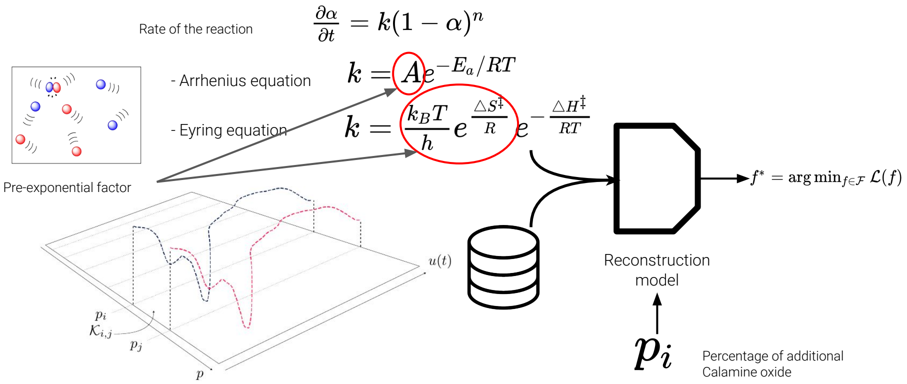


Osmani, Aomar, Hamidi, Massinissa, and Bouhouche, Salah. *Proceedings of the AAAI Conference on Artificial Intelligence* 2021

Synthesis of New Materials in Industry

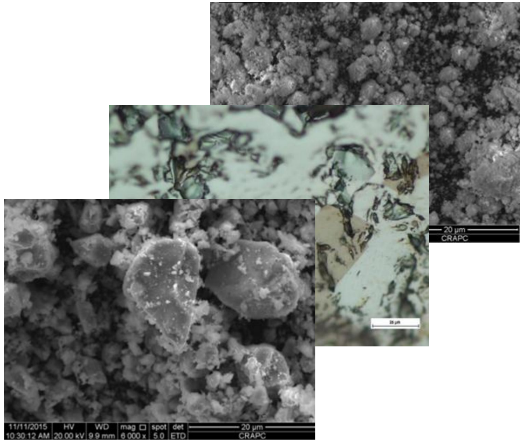
Binary Mixture and Target Material

Calamine Oxide

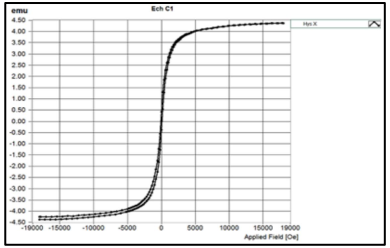
Red Pigment

proportion in %

Synthesis
(Real experiments)



optical properties



ferromagnetic properties

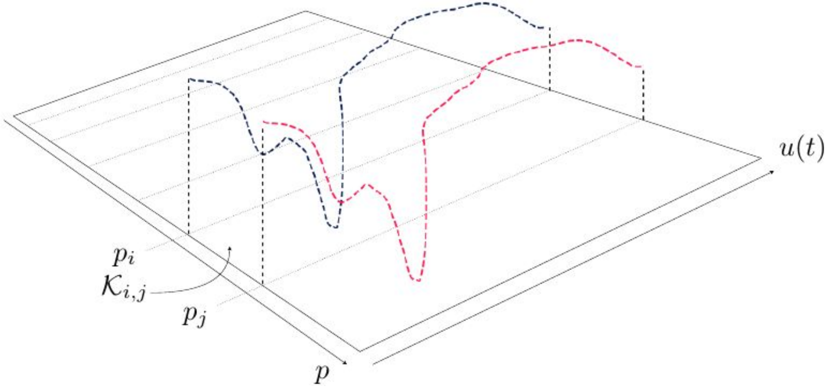
AbedGhars, Mohamed Tayeb. Diss. Université Badji Mokhtar de Annaba, 2018.

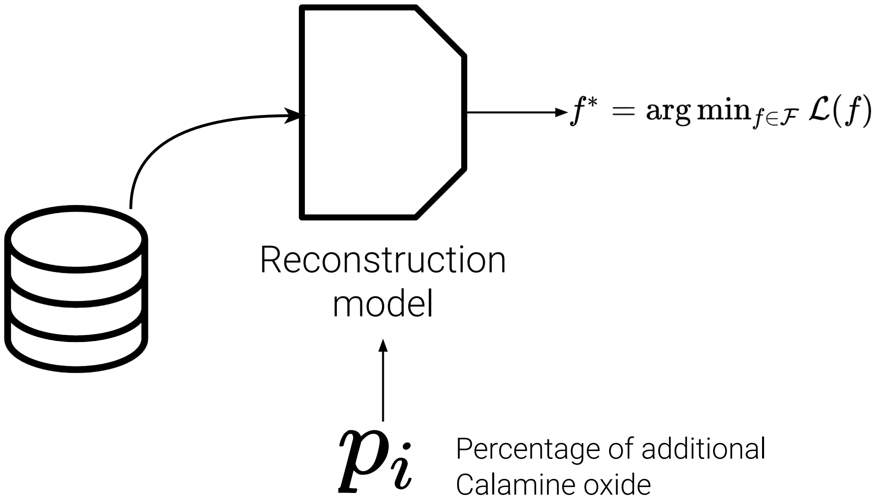
State Space Partitioning & Evaluation Protocol

Reconstruction models:

- Inside circumscribed regions;
- Outside circumscribed regions

State space





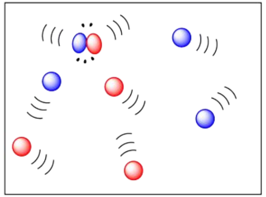
Combining Domain Models & Empirical Data

Combining Analytical Models and Real Experiments

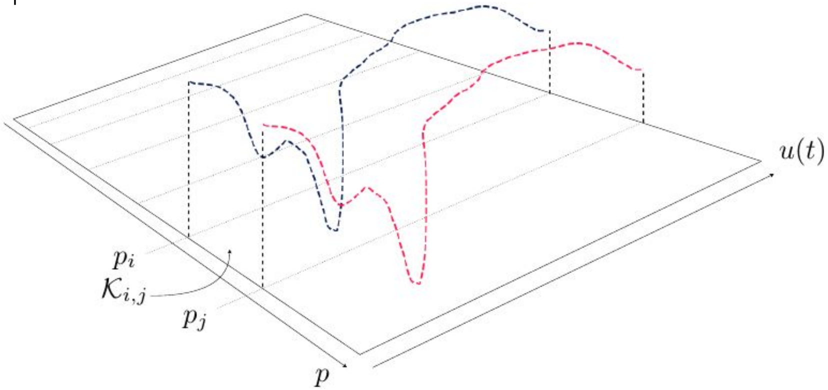
Rate of the reaction $$\frac{\partial \alpha}{\partial t} = k(1-\alpha)^n$$

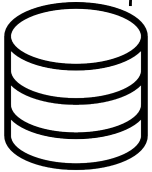
- Arrhenius equation $$k = Ae^{-E_a/RT}$$

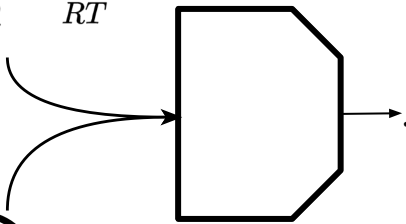
- Eyring equation $$k = \frac{k_B T}{h} e^{\frac{\triangle S^{\ddagger}}{R}} e^{-\frac{\triangle H^{\ddagger}}{RT}}$$



Pre-exponential factor







Reconstruction model

$$f^* = \arg\min_{f \in \mathcal{F}} \mathcal{L}(f) + \lambda R(f)$$

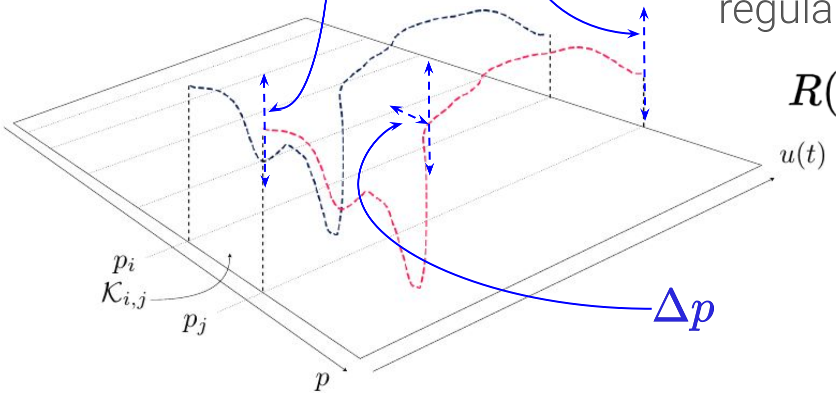
$$p_i$$ Percentage of additional Calamine oxide

Laidler, Keith J. Journal of chemical Education 61.6 (1984): 494.
Lasaga, Antonio C. Rev. Mineral. 8 (1981).

Kinetic-Based Regularization

$$f^* = \arg\min_{f \in \mathcal{F}} \mathcal{L}(f) + \lambda R(f)$$

$$\mathbf{b}_j = [\underline{\Delta_j^{t_1}}, \dots, \underline{\Delta_j^{t_{max}}}]$$



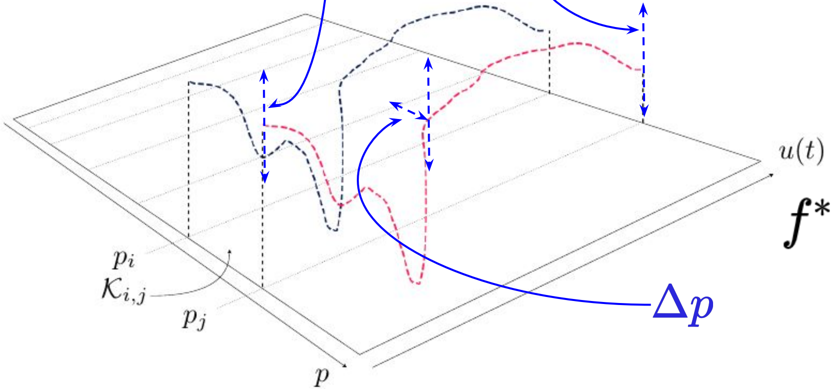
Using the neighboring points $p_i + \Delta p, p_i + 2\Delta p, p_i + 3\Delta p$ we derive a series of penalty bounds $\mathbf{b}_j = [\Delta_j^{t_1}, \dots, \Delta_j^{t_{max}}]$ at each applied temperature $t_1, \dots, t_{max}$. The regularization-like term becomes

$$R(f) = \frac{1}{P} \sum_{j=1}^{P} \mathbb{1}\{|f(p_i + j\Delta p) - \mathbf{b}_j| > \epsilon\}$$

Boyd, Stephen, Stephen P. Boyd, and Lieven Vandenberghe. Cambridge university press, 2004.
Ravi, Sathya N., et al. *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 33. 2019.

Finding Pareto-Optimal Solutions

$$\mathbf{b}_j = [\Delta_j^{t_1}, \ldots, \Delta_j^{t_{max}}]$$



$$f^* = \arg\min_{f \in \mathcal{F}} \mathcal{L}(f) + \lambda R(f)$$

Stochastic
Gradient
Descent

$$f^* = \arg\min_{f \in \mathcal{F}} \mathcal{L}(f) \text{ s.t. } R(f) \leq \mu$$

Conditional
Gradient

Boyd, Stephen, Stephen P. Boyd, and Lieven Vandenberghe. Cambridge university press, 2004.
Ravi, Sathya N., et al. *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 33. 2019.

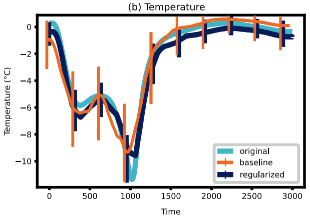
Experiments

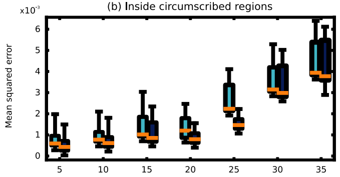
Experimental Setup

- Dataset
    - SDT-Q600 from TA-instruments version 20.9 build 20;
    - Monitored signals: temperature (°C), weight (mg), heat flow (mW), temperature difference(μV), sample purge flow (mL/min), etc.;
    - 3000 measurement points at a sampling rate of 2 Hz;
    - Real experiments conducted at 5, 10, 15, 20, 25, and 35 % of additional calamine oxide
- Training details
    - Stacking of Conv1d/ReLU/MaxPool blocks (Tensorflow);
    - Hyperparameter optimization (scikit-optimize/Microsoft NNI);
    - Kinetics regularization-like terms derived analytically (chempy)

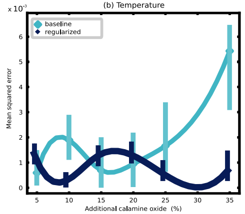
Experimental Evaluation

(i) Reconstruction Process





(ii) Distance between Training and Validation Experiments



(iii) Reconstruction at specific percentages

Analytical model(s)	Reconstruction error avg.±std. $\times 10^{-2}$ (best extent %)			
	$\lambda = 0.001$	$\lambda = 0.01$	$\lambda = 0.1$	$\lambda = 1$
Arrhenius (A)	0.933 ± .0073 (5)	0.988 ± .0023 (15)	**0.39** ± **.0157** (15)	0.776 ± .0027 (5)
Eyring (E)	0.57 ± .0145 (10)	0.385 ± .0031 (5)	**0.228** ± **.0079** (10)	0.587 ± .0037 (**20**)
pig (P)	2.408 ± .0034 (10)	**0.408** ± **.015** (5)	1.188 ± .0061 (5)	2.408 ± .0042 (10)
cala (C)	0.533 ± .0112 (15)	0.512 ± .0055 (**20**)	0.524 ± .0047 (5)	**0.504** ± **.0125** (10)
A+E	**0.188** ± **.0058** (5)	0.197 ± .0079 (**20**)	0.214 ± .0051 (10)	0.204 ± .0147 (15)
P+C	0.318 ± .0012 (5)	**0.289** ± **.0044** (10)	0.309 ± .0108 (10)	0.320 ± .0086 (10)
A+E+P+C	**0.192** ± **.0056** (15)	0.201 ± .0122 (5)	0.247 ± .0032 (10)	0.231 ± .0143 (15)

(iv) Trade-off between real experiments and analytical models

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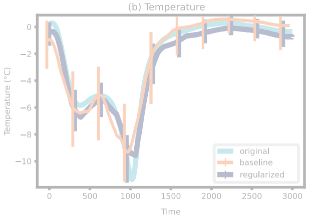

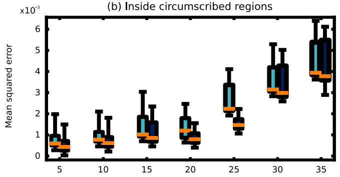

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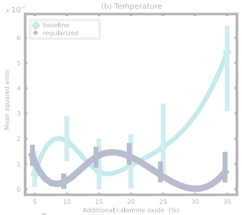

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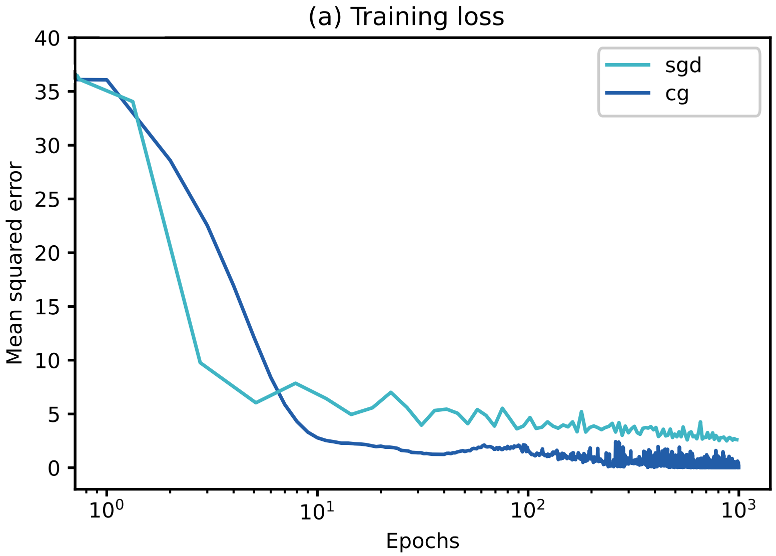

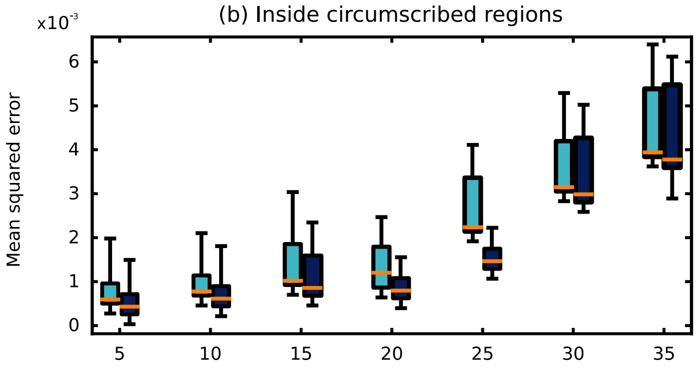

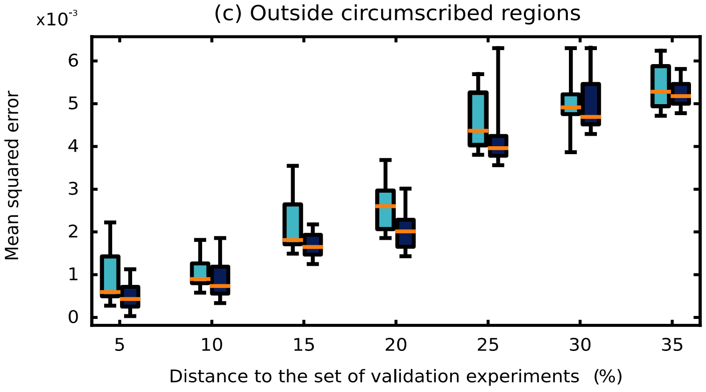

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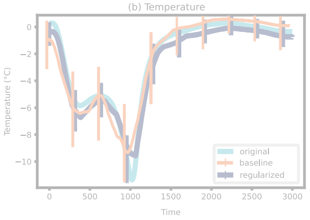

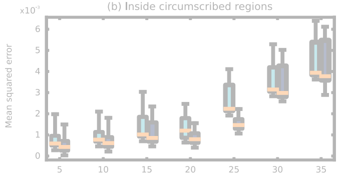

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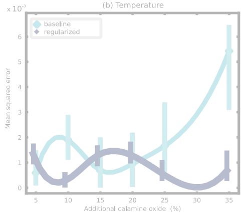

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Arrhenius (A)	0.933 $\pm$ .0073 (5)	0.988 $\pm$ .0023 (15)	**0.39** $\pm$ **.0157** (15)	0.776 $\pm$ .0027 (5)
Eyring (E)	0.57 $\pm$ .0145 (10)	0.385 $\pm$ .0031 (5)	**0.228** $\pm$ **.0079** (10)	0.587 $\pm$ .0037 (**20**)
pig (P)	2.408 $\pm$ .0034 (10)	**0.408** $\pm$ **.015** (5)	1.188 $\pm$ .0061 (5)	2.408 $\pm$ .0042 (10)
cala (C)	0.533 $\pm$ .0112 (15)	0.512 $\pm$ .0055 (**20**)	0.524 $\pm$ .0047 (5)	**0.504** $\pm$ **.0125** (10)
A+E	**0.188** $\pm$ **.0058** (5)	0.197 $\pm$ .0079 (**20**)	0.214 $\pm$ .0051 (10)	0.204 $\pm$ .0147 (15)
P+C	0.318 $\pm$ .0012 (5)	**0.289** $\pm$ **.0044** (10)	0.309 $\pm$ .0108 (10)	0.320 $\pm$ .0086 (10)
A+E+P+C	**0.192** $\pm$ **.0056** (15)	0.201 $\pm$ .0122 (5)	0.247 $\pm$ .0032 (10)	0.231 $\pm$ .0143 (15)

En résumé

- L'internet des objets offre un cadre applicatif très riche pour l'apprentissage ;
- L'IoT permet d'évaluer les modèles sous des hypothèses plus réalistes ;
- L'IoT offre aussi un cadre pour évaluer les aspects réglementaires (santé, vie privée, etc.) liés aux déploiements de capteurs et aux modèles d'apprentissage.

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