Best Practices: Software Engineering, Machine Learning, and AutoML

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Koen van der Blom

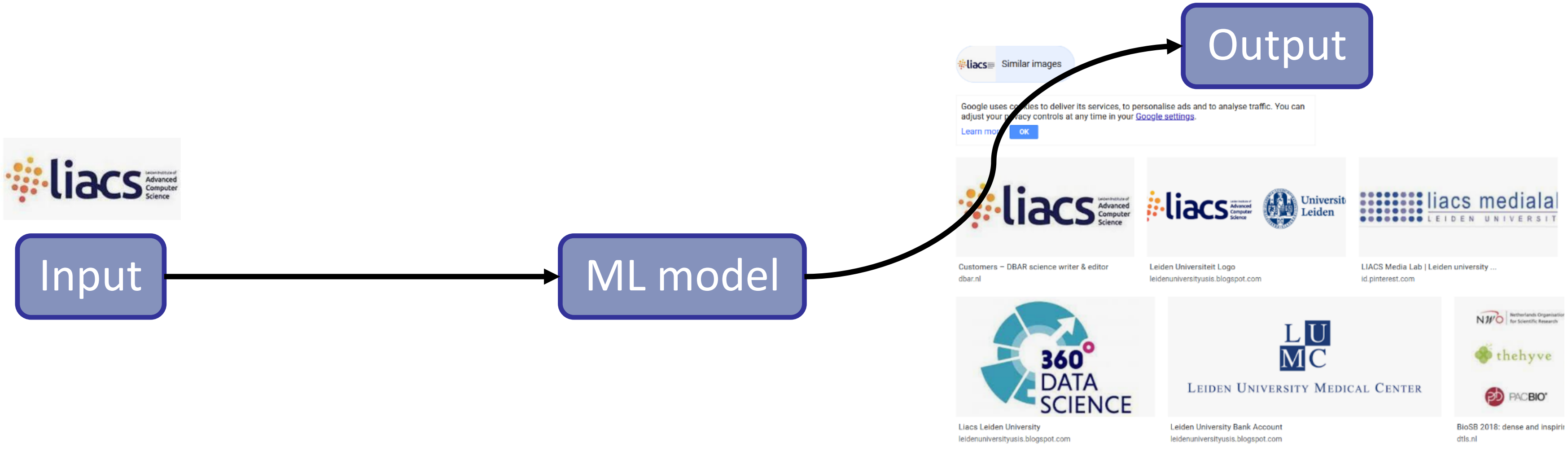
- Background
  - The Hague University of Applied Sciences
    - Bachelor Informatica
  - Leiden University
    - MSc Comp. Sci. → PhD → Postdoc

- Research
  - Meta-algorithmics, automated ML+AI
  - Multi-objective optimisation
  - Evolutionary computation and swarm intelligence
  - Software engineering for ML

Machine learning

- Many techniques
- You learned
  - How they work
  - How you can use them
- Industry ‘real-world’
  - ML as part of a larger system

Image search



(imaginary system)

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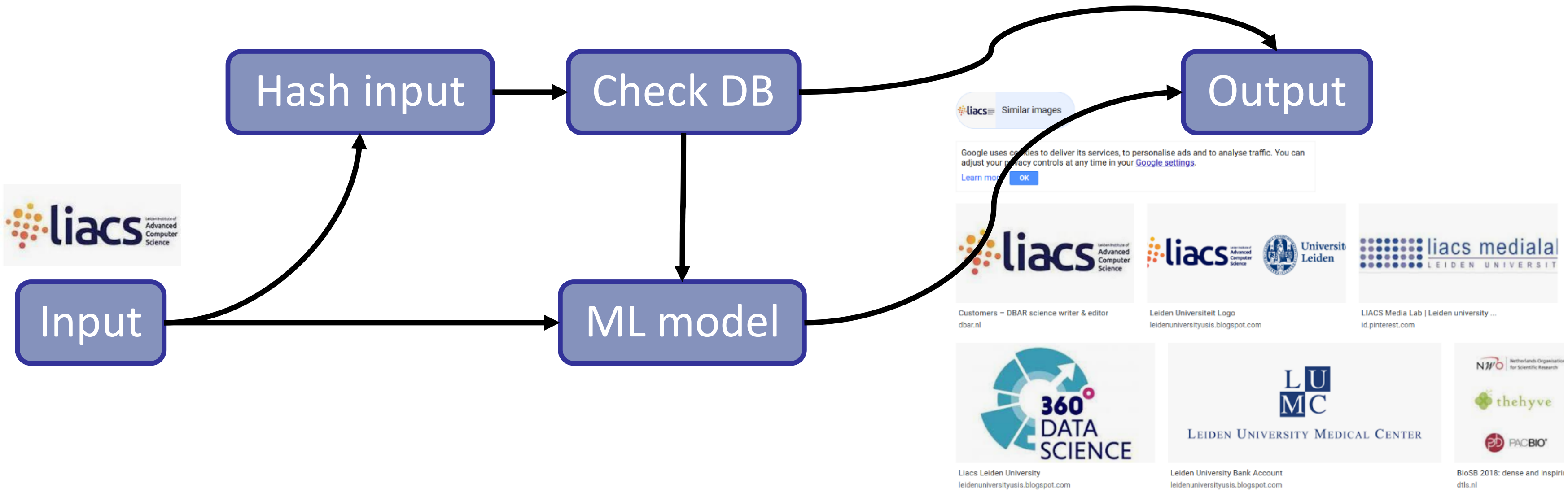

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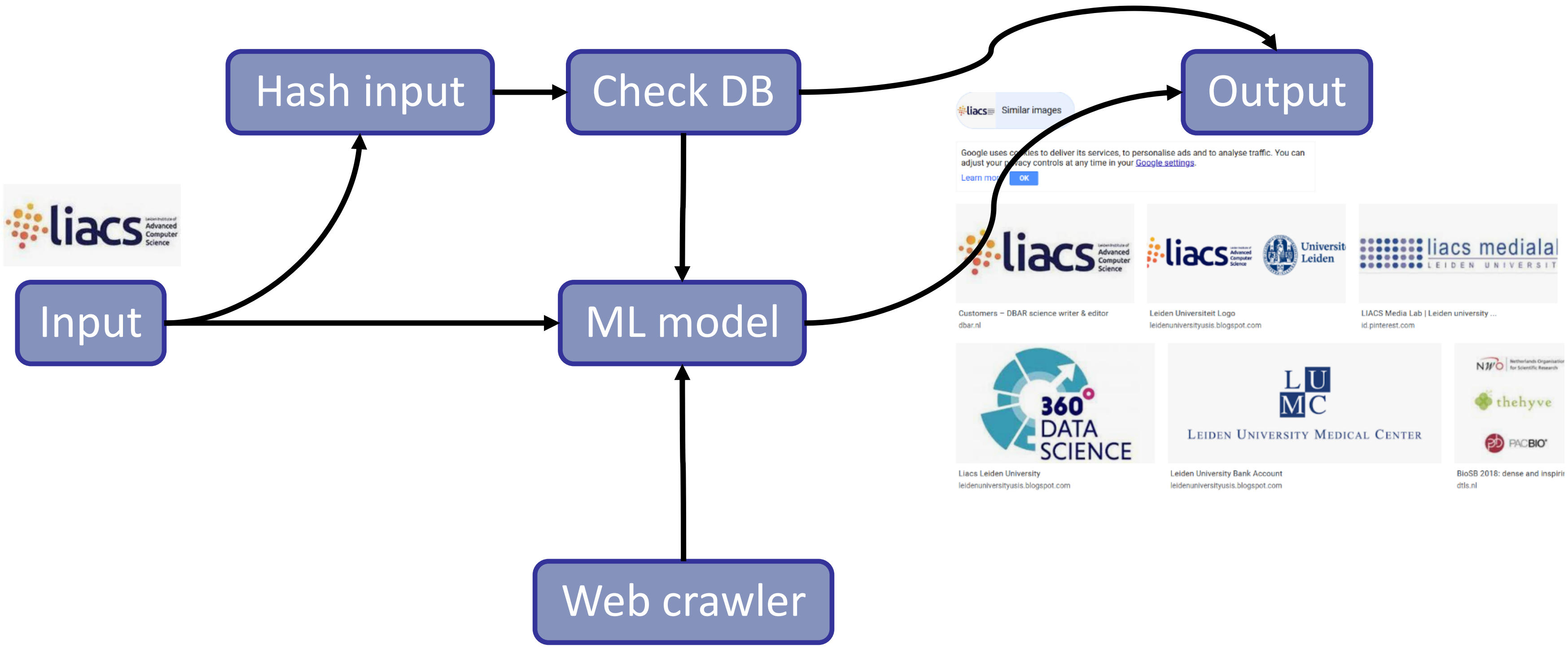

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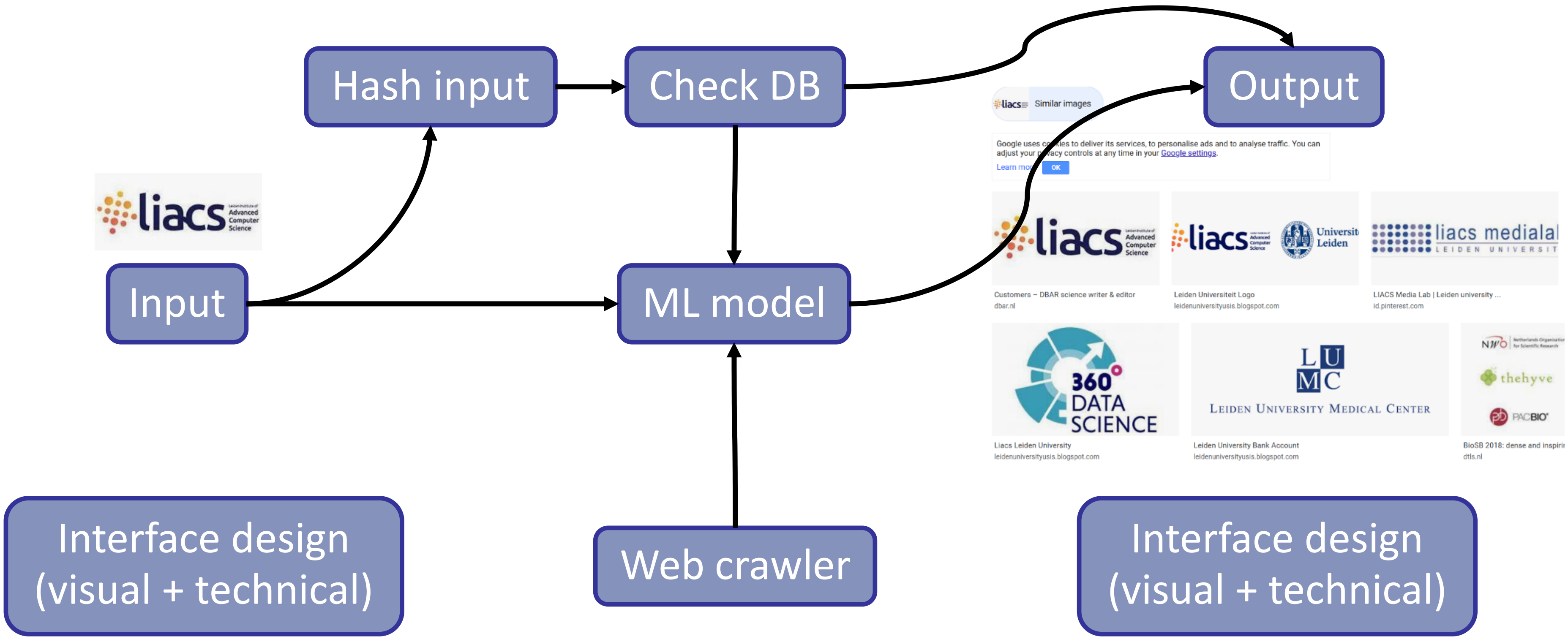

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Image search

- Find (source of) original or similar image
- Input image
  - Did someone look for it before?
    - Check input URL/image;
    - Hash function;
    - Basic/cheap features
  - Yes: Look up in database, done!
  - No: Run through ML model
- Interface: Also part of the system!
  - Receive user input
  - Display results

Engineering software with ML

- Software engineering (SE)
  + Machine learning

- Best practices: Guidelines, can have exceptions!

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- Improve
  - Agility
  - Software quality
  - Team effectiveness
  - Traceability

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- Traceability: Trace work items in the development lifecycle
  - Why did we develop this code?
  - Does it do what we intended?

Best practices for SE

- What do you already know?

Best practices for SE

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- Things that may be familiar
  - Collaborative code management (e.g., git)
  - Testing (unit tests, regression tests)
  - Documentation (comments, diagrams)
  - Development methodology (e.g., agile/scrum)

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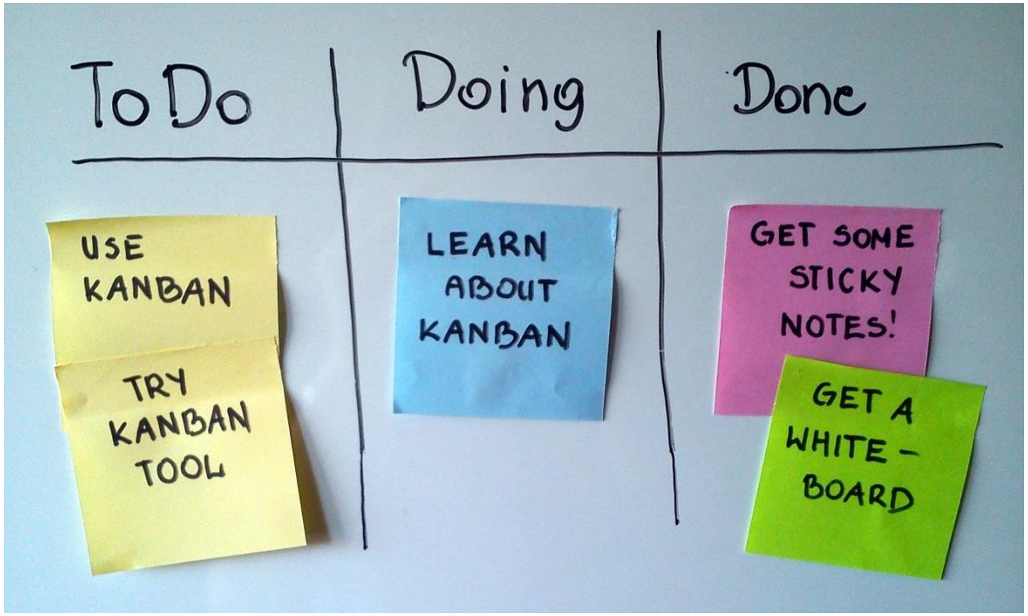

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- Versioning

Software with ML components

- SE with ML is different from just SE
- Do engineering practices still apply?
- Do we have to change practices?
- Do we need new practices?

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- Do we need new practices?
- Yes ...all of those!

Practices that still apply

- Still working with code
  - Automated regression testing → Does it still work?
  - Continuous integration → Automatically build/compile
  - Static analysis → Check code quality

- Still a team effort
  - Collaborative development platform → Integrate changes
  - Use a shared backlog → Task status, priority
  - Communicate → Still working towards the same goal?

Practices that still apply

- Limited attention for these practices in ML

Out of 29

Title	Rank
Run Automated Regression Tests	27
Use Continuous Integration	16
Use Static Analysis to Check Code Quality	24
Use A Collaborative Development Platform	8
Work Against a Shared Backlog	9
Communicate, Align, and Collaborate With Multidisciplinary Team Members	10

From: Serban et al. 2020

- Adopt and you are ahead of the competition!

What is different with ML?

What is different with ML?

- Use data
- Create ML models
- Optimise ML system for accuracy
  - Choose best features
  - Optimise parameter settings
  - Etc.
- Run on new data, from real people…

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- Documentation → What does each feature (property) mean, why does it make sense to use?
- Peer review → Training scripts
- Versioning → Datasets, models, etc.
- Automate → Model deployment, roll backs
- Logging → Every prediction a model makes, including version numbers and input data

New practices

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- Share data sets → ensure everyone works on the same

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- Remove or archive unused features
- Enable parallel training experiments
- Share experimental results → Avoid repetition
- Monitor deployed models

Automated machine learning

- Feature generation
- Feature selection

- Model selection
- Algorithm selection

- Hyperparameter optimisation

- Algorithm configuration
- Neural architecture search

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but all automated!

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…and more

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- Which model/algorithm to choose?
- Best is not always the same
  - Even with relatively small changes!
- Manually run things, see what works where

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- Or: Automated ML system

- E.g., Automate choice of model to deploy

- Predict which model to use for which input

Automated tuning / configuration

- Which settings/parameters to use?
- Which algorithm/model architecture works best?
- Difficult to know what works well
  - Try many things → takes a lot of human time
  - Find improvements → but is it really the best?

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- Or: Automated ML system
- E.g. Neural architecture search
  - Optimised (deep) neural network for our use case

All is well then, …or is it?

- Can we trust the system?
- Uses data, but which data, and how?
- Are the results biased?
- Do the users know it is an ML system, can they raise concerns when things go wrong?
- Can we explain why the ML system does what it does?

Trustworthy ML

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- Use privacy preserving ML techniques
  - E.g., federated learning

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  - Data
  - Manipulation of system behaviour

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  - Manipulation of system behaviour
- Perform risk assessments
- Provide audit trails
- Have your application audited

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  - What does it mean to be responsible?

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- Establish responsible AI values
  - What does it mean to be responsible?
- Use interpretable models whenever possible
- Use team process for decision making
  - Higher accuracy ‘blackbox’ model or slightly less accurate interpretable model?
  - E.g., When do we accept a blackbox model?

Trustworthy ML

- Inform users about ML usage

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- Provide safe channels to raise concerns

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- Provide safe channels to raise concerns
- Explain results and decisions to users

Many practices, where to start?

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- Aim: Rank by difficulty (work in progress)

Use Versioning for Data, Model, Configurations and Training Scripts	Training	basic
Share Status and Outcomes of Experiments Within the Team	Training	basic
Run Automated Regression Tests	Coding	advanced
Use Continuous Integration	Coding	medium
Use Static Analysis to Check Code Quality	Coding	advanced

Summary

- SE for ML is still SE
  - Don’t abandon best practices
  - Adapt and extend them
- AutoML to maximise performance
- Build a system we can trust
- Learn more: https://se-ml.github.io