MAKE Decisions Medical Information Science for Decision Support





Assoc. Prof. Dr. Andreas HOLZINGER (Medical University Graz)

https://hci-kdd.org/mini-course-make-decisions-practice

Day 1 > Part 1 > 19.09.2018

Information Sciences meets Life Sciences

Andreas Holzinger: Background



- PhD in Cognitive Science 1998
- Habilitation Computer Science 2003
- Lead Holzinger Group HCI-KDD www.hci-kdd.org
- Visiting Professor for Machine Learning in Health Informatics: TU Vienna, Univ. Verona, UCL London, RWTH Aachen
- Research Statement see: Holzinger, A. (2016) Interactive Machine Learning for Health Informatics: When do we need the human-in-the-loop? Springer Brain Informatics, 3, 1-13, doi:10.1007/s40708-016-0042-6
- Most recent: Holzinger, A. 2018. Explainable AI (ex-AI). Informatik-Spektrum, doi:10.1007/s00287-018-1102-5



Mini-Course Syllabus



- At the end of this course you will ...
- ... be fascinated to see our world in data sets;
- ... understand the differences between data, information and knowledge
- ... be aware of some problems and challenges in biomedical informatics
- ... understand the importance of the concept of probabilistic information p(x)
- ... know what AI/Machine Learning can (not) do
- ... have some fundamental insight into medical information science for decision making

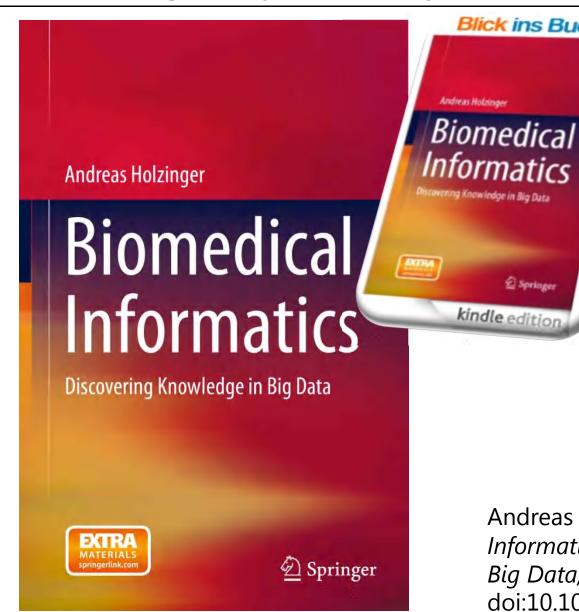
Reading on Paper or on any electronic device

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2 Springer

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Andreas Holzinger 2014. Biomedical Informatics: Discovering Knowledge in Big Data, New York, Springer, doi:10.1007/978-3-319-04528-3.

Overview



Primer on Probability & Information

Day 1 - Fundamentals

Day 2 – Hot Topics

01 Information Sciences meets Life Sciences

05 Methods of Explainable-AI

02 Data, Information and Knowledge



Groupwork: Planning of a 500 bed Hospital - Bringing Al into the workflows

03 Decision Making and Decision Support



04 From Expert Systems to Explainable AI

Plenary: Presenting the developed concepts



- 01 What is the HCI-KDD approach?
- 02 Application Area: Health Informatics
- 03 Probabilistic Information
- 04 Automatic Machine Learning
- 05 Interactive Machine Learning
- 06 Key Problems in Biomedical Informatics



01 What is the



approach?



ML is a very practical field – algorithm development is at the core however, successful ML needs a concerted effort of various topics ...





Andreas Holzinger 2017. Introduction to Machine Learning and Knowledge Extraction (MAKE). *Machine Learning and Knowledge Extraction*, 1, (1), 1-20, doi:10.3390/make1010001.

Cognitive Science AND Computer Science





- Cognitive Science → human intelligence
- Computer Science → computational intelligence
- Human-Computer Interaction → the bridge

Andreas Holzinger 2013. Human—Computer Interaction and Knowledge Discovery (HCI-KDD): What is the benefit of bringing those two fields to work together? In: Springer Lecture Notes in Computer Science LNCS 8127. Heidelberg, Berlin, New York: Springer, pp. 319-328, doi:10.1007/978-3-642-40511-2_22.

- 1) learn from prior data
- 2) extract knowledge
- 3) generalize, i.e. guessing where a probability mass function concentrates
- 4) fight the curse of dimensionality
- 5) disentangle underlying explanatory factors of data, i.e.
- understand the data in the context of an application domain



"Solve intelligence – then solve everything else"



https://youtu.be/XAbLn66iHcQ?t=1h28m54s

Demis Hassabis, 22 May 2015

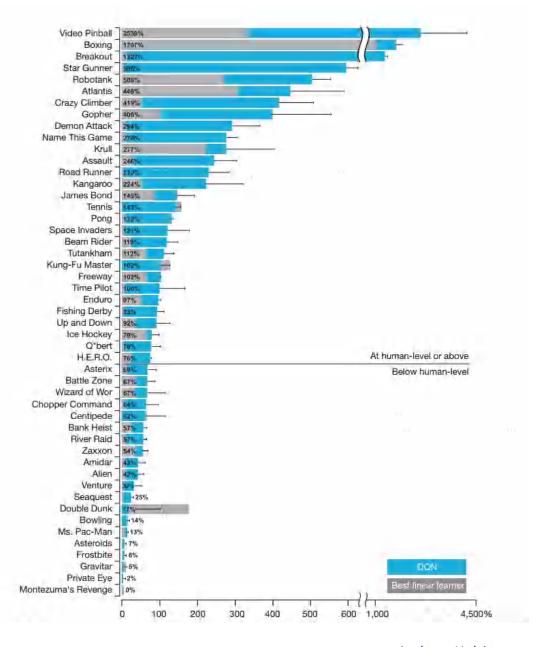
The Royal Society, Future Directions of Machine Learning Part 2





Compare your best ML algorithm with a seven year old child ...

Mnih, V., Kavukcuoglu, K., Silver, D., Rusu, A. A., Veness, J., Bellemare, M. G., Graves, A., Riedmiller, M., Fidjeland, A. K., Ostrovski, G., Petersen, S., Beattie, C., Sadik, A., Antonoglou, I., King, H., Kumaran, D., Wierstra, D., Legg, S. & Hassabis, D. 2015. Human-level control through deep reinforcement learning. Nature, 518, (7540), 529-533, doi:10.1038/nature14236



Not our Goal: Humanoid Al











Why is this application area complex?









Our central hypothesis: Information may bridge this gap

Holzinger, A. & Simonic, K.-M. (eds.) 2011. *Information Quality in e-Health. Lecture Notes in Computer Science LNCS 7058, Heidelberg, Berlin, New York: Springer.*





Main problems ...



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Holzinger, A., Dehmer, M. & Jurisica, I. 2014. Knowledge Discovery and interactive Data Mining in Bioinformatics - State-of-the-Art, future challenges and research directions. BMC Bioinformatics, 15, (S6), I1.



03 Probabilistic Information p(x)

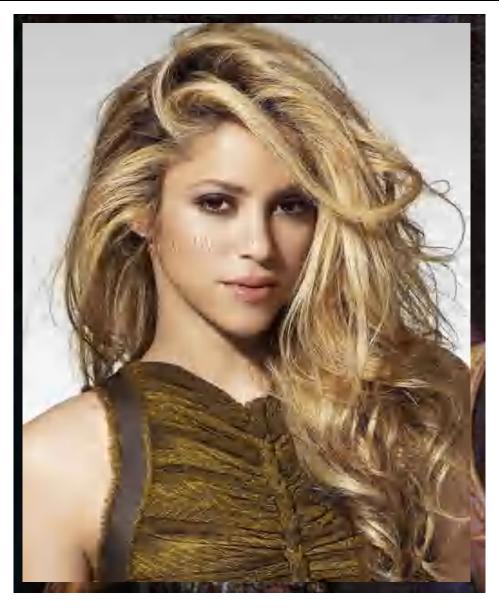
The true logic of this world is in the calculus of probabilities.

James Clerk Maxwell





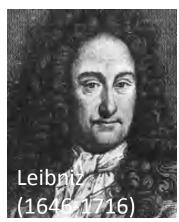
Probability theory is nothing but common sense reduced to calculation



Pierre Simon de Laplace (1749-1827)

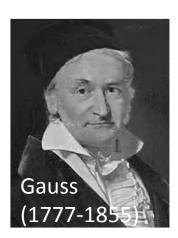












- Newton, Leibniz, ... developed calculus mathematical language for describing and dealing with rates of change
- Bayes, Laplace, ... developed probability theory - the mathematical language for describing and dealing with uncertainty
- Gauss generalized those ideas

Learning representations (θ, h) from observed data



Observed data:



$$pprox$$
 Training data: $\mathcal{D}=x_{1:n}=\{x_1,x_2,...,x_n\}$

Feature Parameter:

 θ

or hypothesis h

 $h \in \mathcal{H}$

Prior belief pprox prior probability of hypothesis h: $p(\theta)$ p(h)

Likelihood $\approx p(x)$ of the data that h is true $p(\mathcal{D}|\theta) = p(d|h)$

Data evidence pprox marginal p(x) that h = true $p(\mathcal{D})$ $\sum_{h \in \mathcal{H}} p(d|h) * p(h)$

Posterior $\approx p(x)$ of h after seen ("learn") data d $p(\theta|\mathcal{D})$ p(h|d)

$$posterior = \frac{likelihood * prior}{evidence} p(\theta | \mathcal{D}) = \frac{p(\mathcal{D} | \theta) * p(\theta)}{p(\mathcal{D})}$$

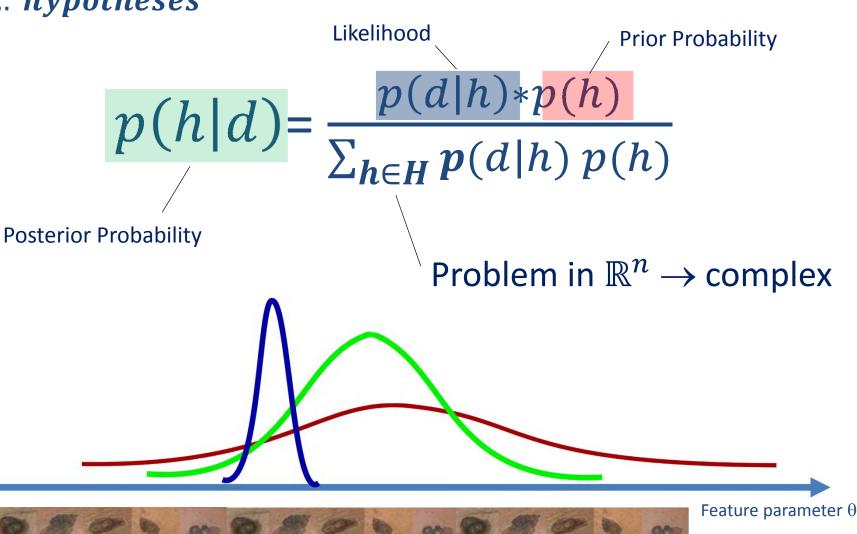
$$p(h|d) = \frac{p(d|h) * p(h)}{\sum_{h \in \underline{H}} p(d|h) p(h)}$$

04

d ... data

$$\mathcal{H} \{H_1, H_2, ..., H_n\} \quad \forall h, d$$

h ... hypotheses





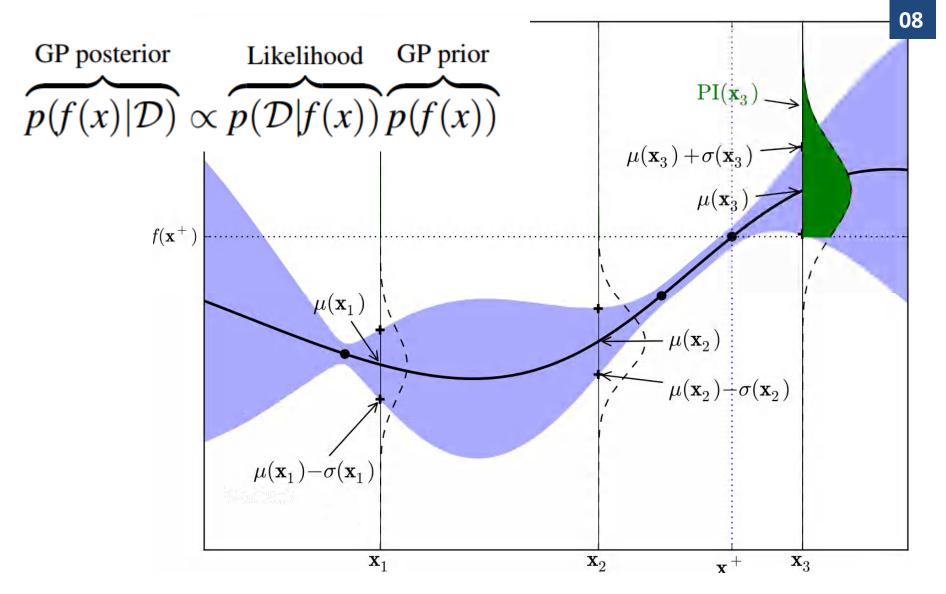
Why is this relevant for health informatics?

Reasoning under uncertainty: Decision Making



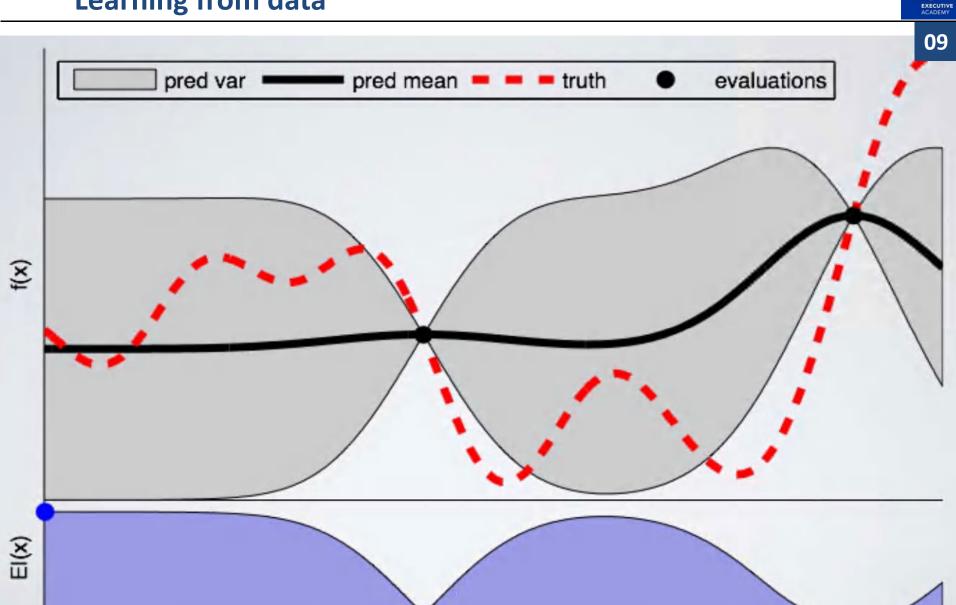
- Take patient information, e.g., observations, symptoms, test results, -omics data, etc. etc.
- Reach conclusions, and predict into the future,
 e.g. how likely will the patient be ...
- Prior = belief before making a particular observation
- Posterior belief after making the observation and is the prior for the next observation – intrinsically incremental

$$p(x_i|y_j) = \frac{p(y_j|x_i)\overline{p}(x_i)}{\sum p(x_i, y_j)p(x_i)}$$



Brochu, E., Cora, V. M. & De Freitas, N. 2010. A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. arXiv:1012.2599.

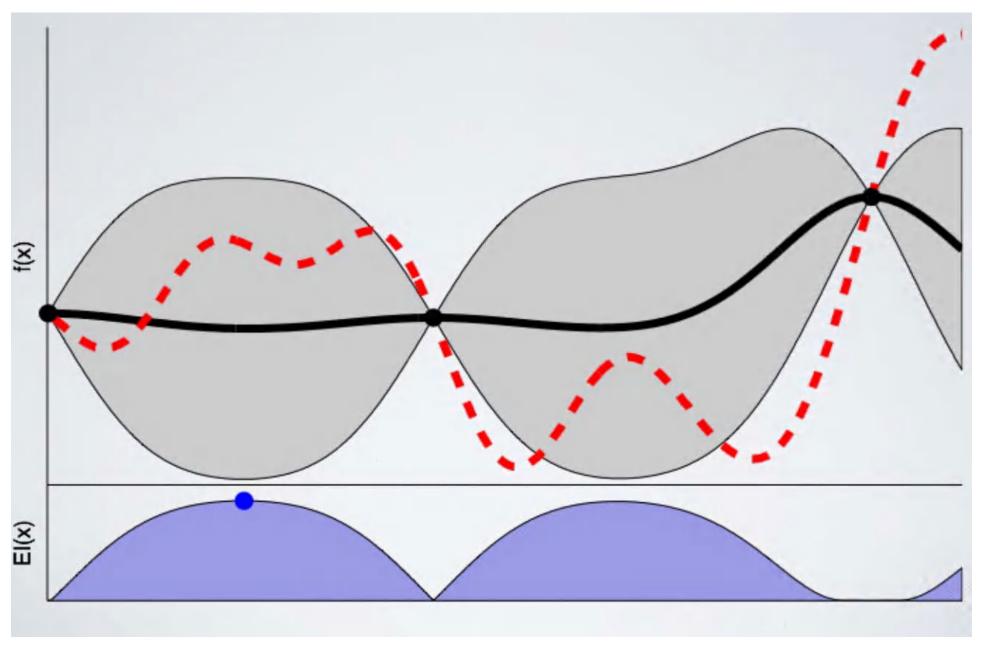
Learning from data



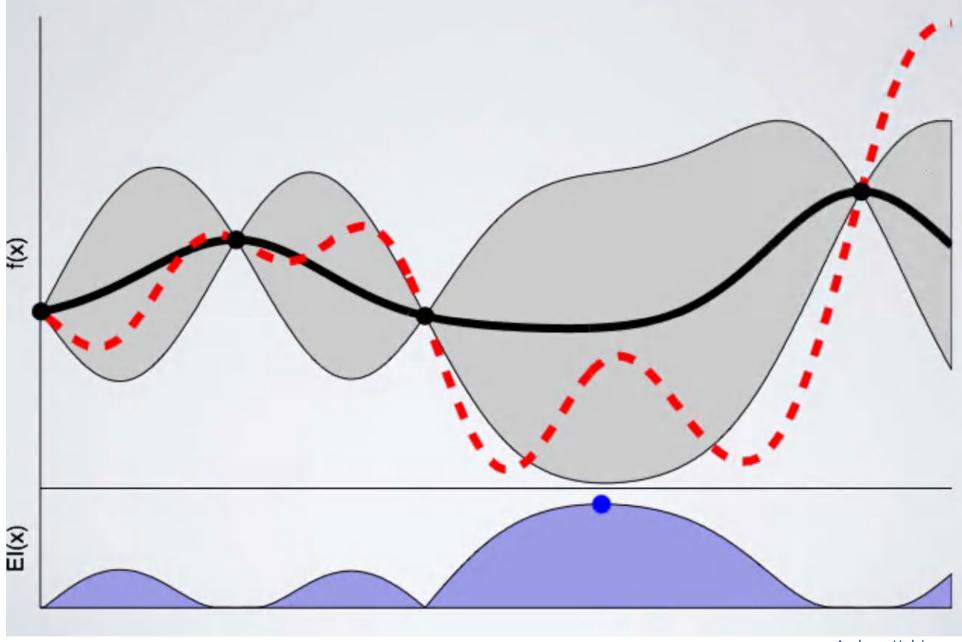
Snoek, J., Larochelle, H. & Adams, R. P. Practical Bayesian optimization of machine learning algorithms. Advances in neural information processing systems, 2012. 2951-2959.

Andreas Holzinger **Health Informatics** 28

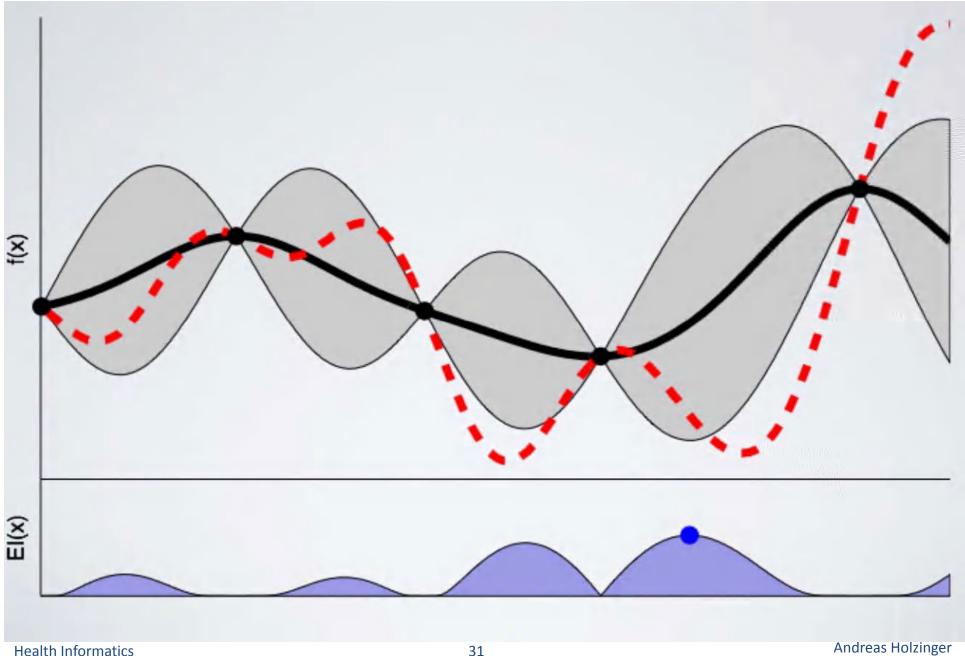




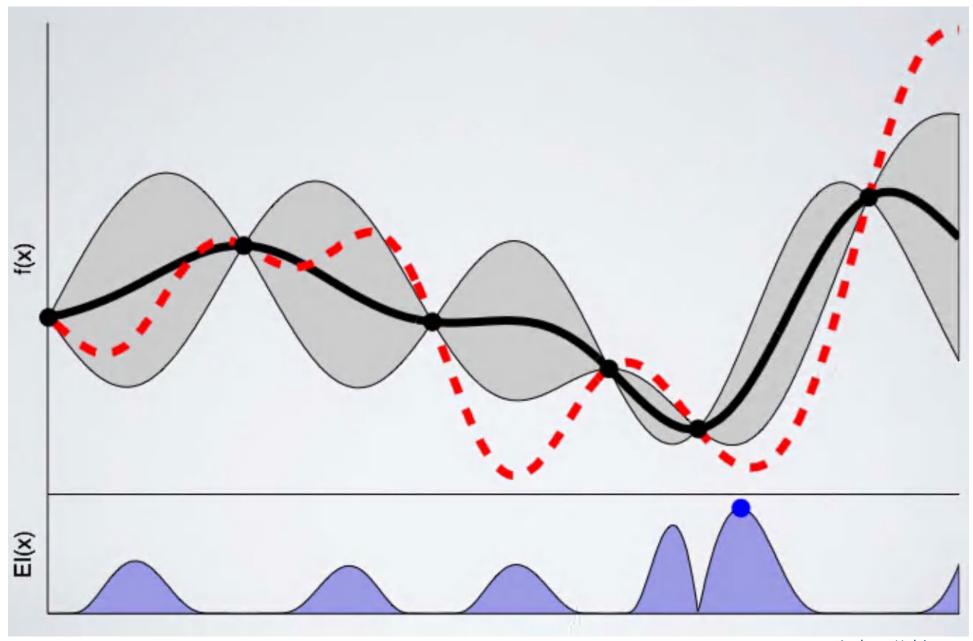




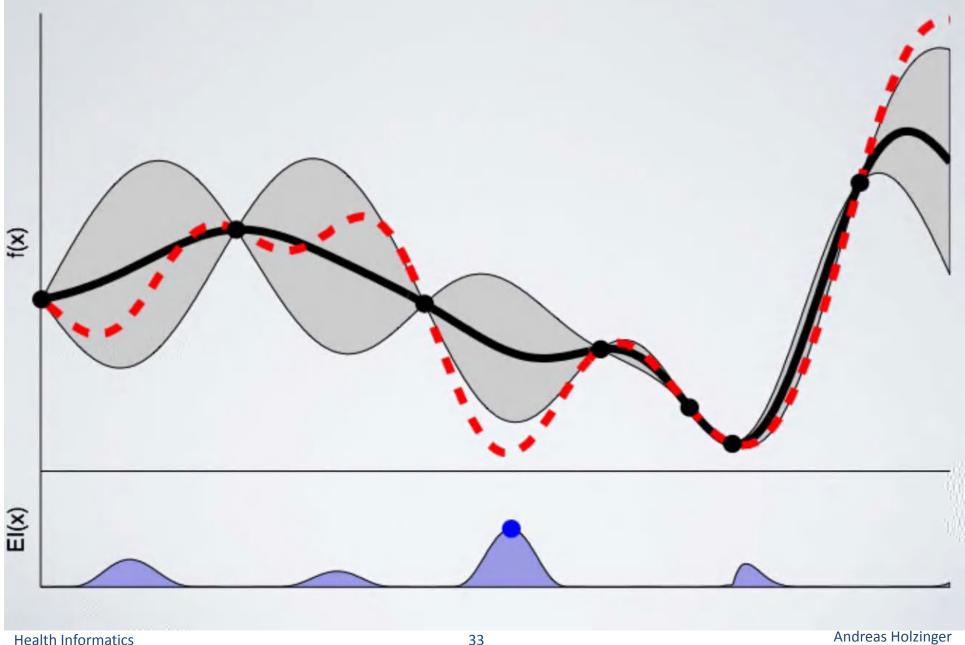




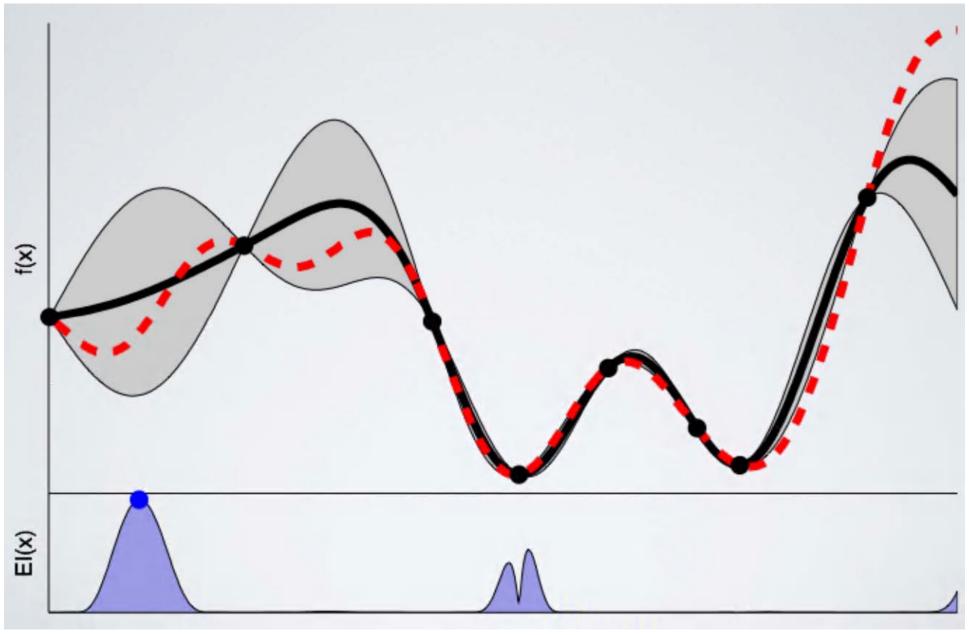


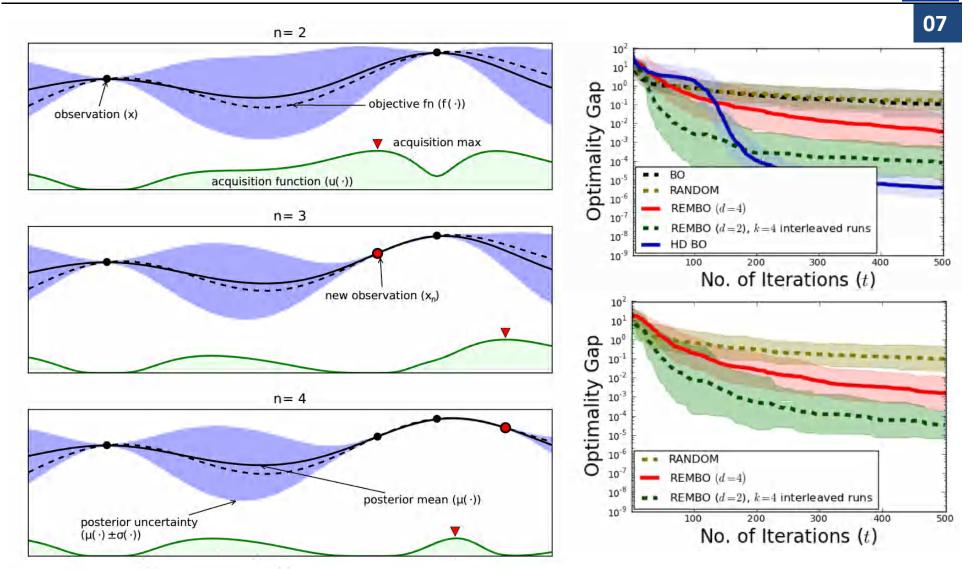






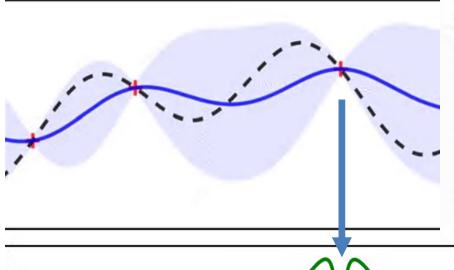






Wang, Z., Hutter, F., Zoghi, M., Matheson, D. & De Feitas, N. 2016. Bayesian optimization in a billion dimensions via random embeddings. Journal of Artificial Intelligence Research, 55, 361-387, doi:10.1613/jair.4806.

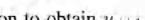
07



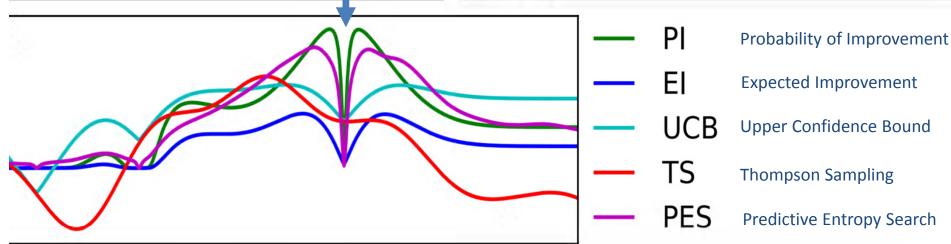
Algorithm 1 Bayesian optimization

- 1: **for** $n = 1, 2, \dots$ **do**
- select new x_{n+1} by optimizing acquisition function α

$$\mathbf{x}_{n+1} = \operatorname*{arg\,max}_{\mathbf{x}} \, \alpha(\mathbf{x}; \mathcal{D}_n)$$



- query objective function to obtain y_{n+1}
- augment data $\mathcal{D}_{n+1} = \{\mathcal{D}_n, (\mathbf{x}_{n+1}, y_{n+1})\}$
- update statistical model
- 6: end for



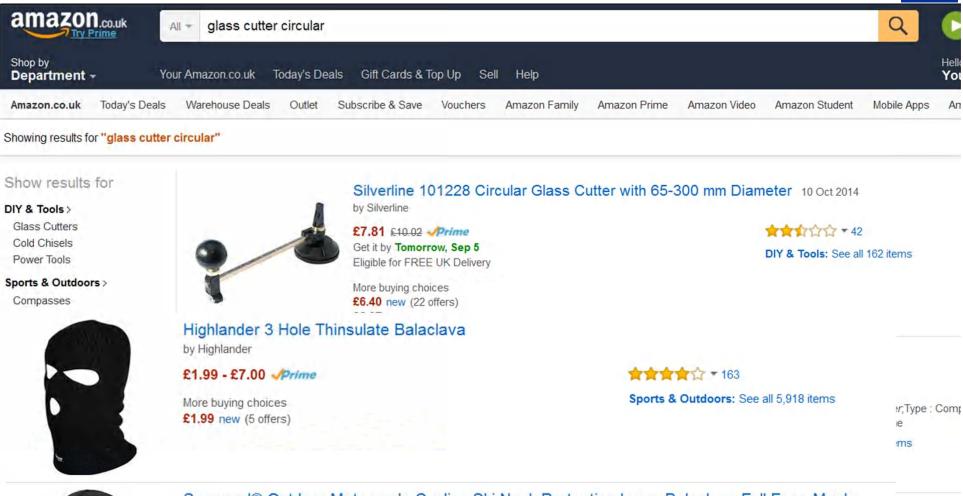
Shahriari, B., Swersky, K., Wang, Z., Adams, R. P. & De Freitas, N. 2016. Taking the human out of the loop: A review of Bayesian optimization. Proceedings of the IEEE, 104, (1), 148-175, doi:10.1109/JPROC.2015.2494218.



04 aML

Example for aML: Recommender Systems







Sanwood® Outdoor Motorcycle Cycling Ski Neck Protecting Lycra Balaclava Full Face Mask

by Phoenix B2C UK

£1.74 - £3.57

More buying choices £0.01 new (4 offers)

★★★★ + 73

Sports & Outdoors: See all 5,918 items

Fully automatic autonomous vehicles (Google car)

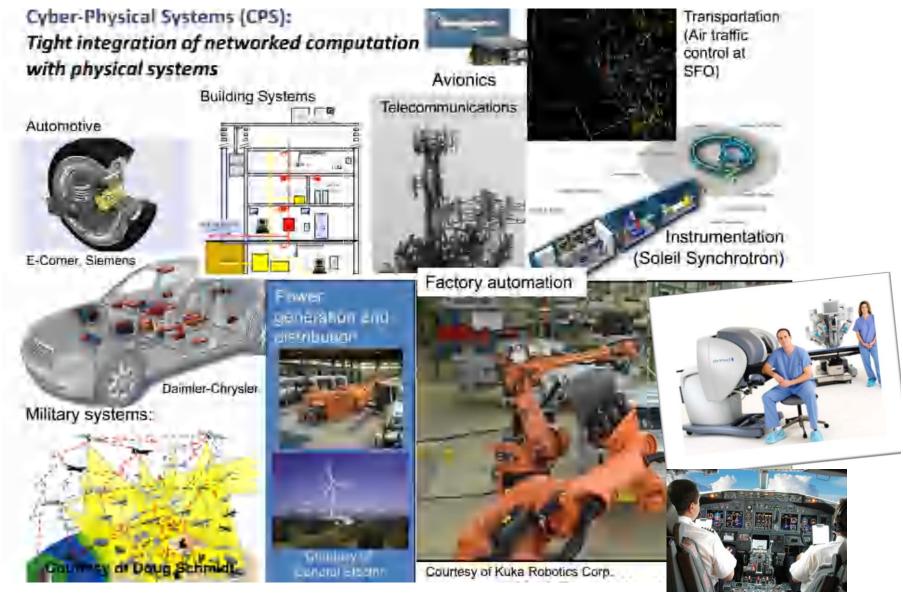




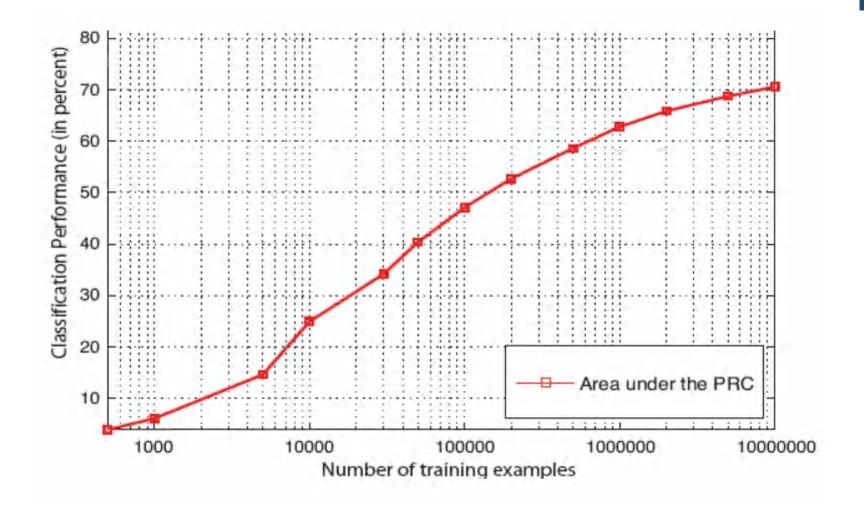
Dietterich, T. G. & Horvitz, E. J. 2015. Rise of concerns about AI: reflections and directions. Communications of the ACM, 58, (10), 38-40.

... and thousands of industrial aML applications ...





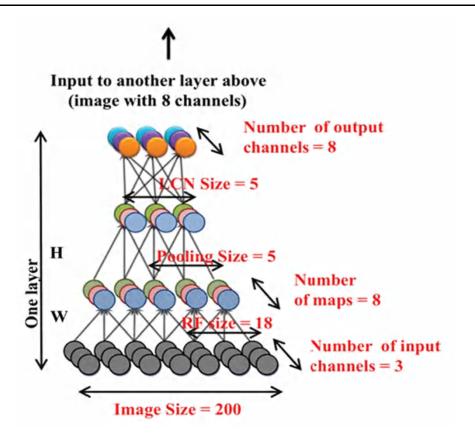
Seshia, S. A., Juniwal, G., Sadigh, D., Donze, A., Li, W., Jensen, J. C., Jin, X., Deshmukh, J., Lee, E. & Sastry, S. 2015. Verification by, for, and of Humans: Formal Methods for Cyber-Physical Systems and Beyond. Illinois ECE Colloquium.



Sonnenburg, S., Rätsch, G., Schäfer, C. & Schölkopf, B. 2006. Large scale multiple kernel learning. Journal of Machine Learning Research, 7, (7), 1531-1565.

10 million 200 χ 200 px images downloaded from Web







$$x^* = \arg\min_{x} f(x; W, H)$$
, subject to $||x||_2 = 1$.

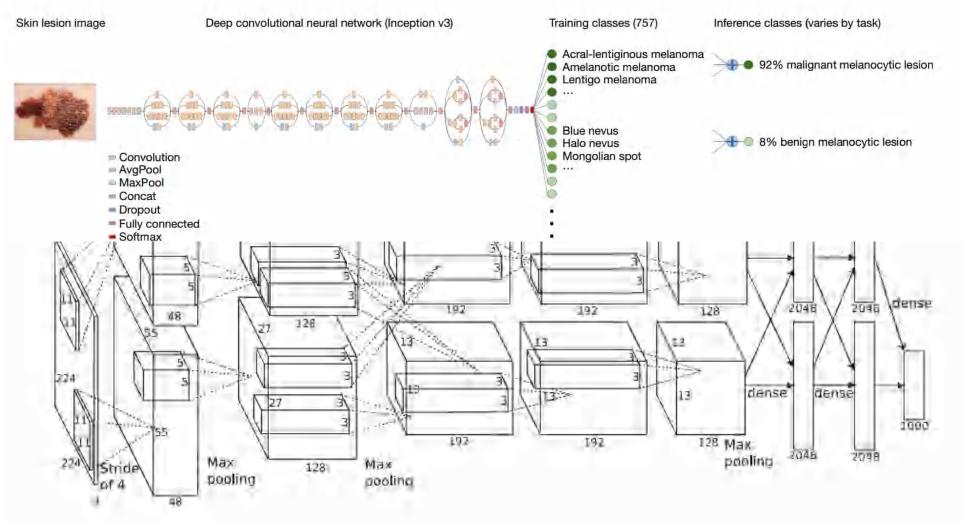
Le, Q. V., Ranzato, M. A., Monga, R., Devin, M., Chen, K., Corrado, G. S., Dean, J. & Ng, A. Y. 2011. Building high-level features using large scale unsupervised learning. arXiv preprint arXiv:1112.6209.

Le, Q. V. 2013. Building high-level features using large scale unsupervised learning. *IEEE Intl. Conference on Acoustics, Speech and Signal Processing ICASSP.* IEEE. 8595-8598, doi:10.1109/ICASSP.2013.6639343.

Deep Convolutional Neural Network Pipeline



Esteva, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M. & Thrun, S. 2017. Dermatologist-level classification of skin cancer with deep neural networks. Nature, 542, (7639), 115-118, doi:10.1038/nature21056.



Krizhevsky, A., Sutskever, I. & Hinton, G. E. Imagenet classification with deep convolutional neural networks. In: Pereira, F., Burges, C. J. C., Bottou, L. & Weinberger, K. Q., eds. Advances in neural information processing systems (NIPS 2012), 2012 Lake Tahoe. 1097-1105.

Limitations of Deep Learning approaches



- Computational resource intensive (supercomps, cloud CPUs, federated learning, ...)
- Black-Box approaches lack transparency, do not foster trust and acceptance among end-user, legal aspects make "black box" difficult!
- Non-convex: difficult to set up, to train, to optimize, needs a lot of expertise, error prone
- Very bad in dealing with uncertainty
- Data intensive, needs often millions of training samples ...



- Sometimes we do not have "big data", where aML-algorithms benefit.
- Sometimes we have
 - Small amount of data sets
 - Rare Events no training samples
 - NP-hard problems, e.g.
 - Subspace Clustering,
 - k-Anonymization,
 - Protein-Folding, ...

Holzinger, A. 2016. Interactive Machine Learning for Health Informatics: When do we need the human-in-the-loop? Springer Brain Informatics (BRIN), 3, (2), 119-131, doi:10.1007/s40708-016-0042-6.



Sometimes we (still) need a human-in-the-loop



05 iML

- iML := algorithms which interact with agents*) and can optimize their learning behaviour through this interaction
- *) where the agents can be human

Holzinger, A. 2016. Interactive Machine Learning (iML). Informatik Spektrum, 39, (1), 64-68, doi:10.1007/s00287-015-0941-6.

Sometimes we need a doctor-in-the-loop





A group of experts-in-the-loop





A crowd of people-in-the-loop

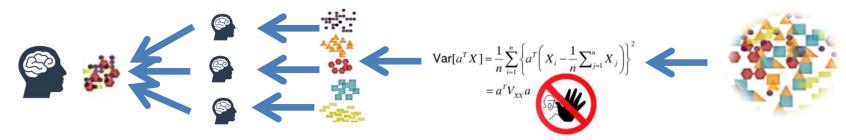




aML: taking the human-out-of-the-loop



A) Unsupervised ML: Algorithm is applied on the raw data and learns fully automatic – Human can check results at the end of the ML-pipeline



B) Supervised ML: Humans are providing the labels for the training data and/or select features to feed the algorithm to learn – the more samples the better – Human can check results at the end of the ML-pipeline



C) Semi-Supervised Machine Learning: A mixture of A and B – mixing labeled and unlabeled data so that the algorithm can find labels according to a similarity measure to one of the given groups











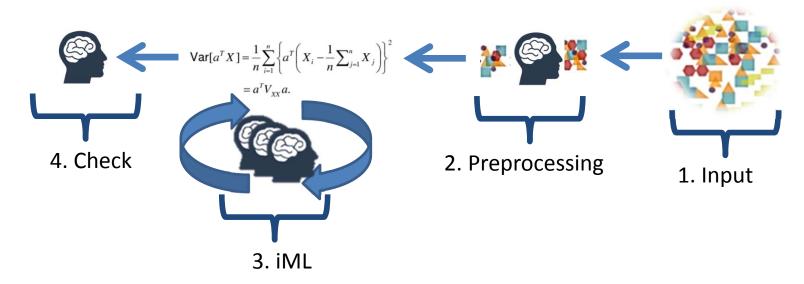








D) Interactive Machine Learning: Human is seen as an agent involved in the actual learning phase, step-by-step influencing measures such as distance, cost functions ...



Constraints of humans: Robustness, subjectivity, transfer? **Open Questions:** Evaluation, replicability, ...

Holzinger, A. 2016. Interactive Machine Learning for Health Informatics: When do we need the human-in-the-loop? Brain Informatics (BRIN), 3, (2), 119-131, doi:10.1007/s40708-016-0042-6.



Example 1: Subspace Clustering

Example 2: k-Anonymization

Example 3: Protein Design

Hund, M., Böhm, D., Sturm, W., Sedlmair, M., Schreck, T., Ullrich, T., Keim, D. A., Majnaric, L. & Holzinger, A. 2016. Visual analytics for concept exploration in subspaces of patient groups: Making sense of complex datasets with the Doctor-in-the-loop. Brain Informatics, 1-15, doi:10.1007/s40708-016-0043-5.

Kieseberg, P., Frühwirt, P., Weippl, E. & Holzinger, A. 2015. Witnesses for the Doctor in the Loop. In: Guo, Y., Friston, K., Aldo, F., Hill, S. & Peng, H. (eds.) Lecture Notes in Artificial Intelligence LNAI 9250. Springer, pp. 369-378, doi:10.1007/978-3-319-23344-4 36.

Lee, S. & Holzinger, A. 2016. Knowledge Discovery from Complex High Dimensional Data. In: Michaelis, S., Piatkowski, N. & Stolpe, M. (eds.) Solving Large Scale Learning Tasks. Challenges and Algorithms, Lecture Notes in Artificial Intelligence LNAI 9580. Springer, pp. 148-167, doi:10.1007/978-3-319-41706-6_7.



06 Key Problems in health informatics



- Zillions of different biological species (humans, animals, bacteria, virus, plants, ...);
- Enormous complexity of the medical domain [1];
- Complex, heterogeneous, high-dimensional, big data in the life sciences [2];
- Limited time, e.g. a medical doctor in a public hospital has only 5 min. to make a decision [3];
- Limited computational power in comparison to the complexity of life (and the natural limitations of the Von-Neumann architecture, ...);
- 1. Patel VL, Kahol K, & Buchman T (2011) Biomedical Complexity and Error. J. Biomed. Inform. 44(3):387-389.
- 2. Holzinger A, Dehmer M, & Jurisica I (2014) Knowledge Discovery and interactive Data Mining in Bioinformatics State-of-the-Art, future challenges and research directions. BMC Bioinformatics 15(S6):I1.
- 3. Gigerenzer G (2008) Gut Feelings: Short Cuts to Better Decision Making (Penguin, London).





Two thematic mainstreams in dealing with data ...



Time

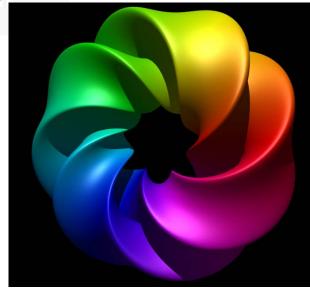
e.g. Entropy



e.g. Topology



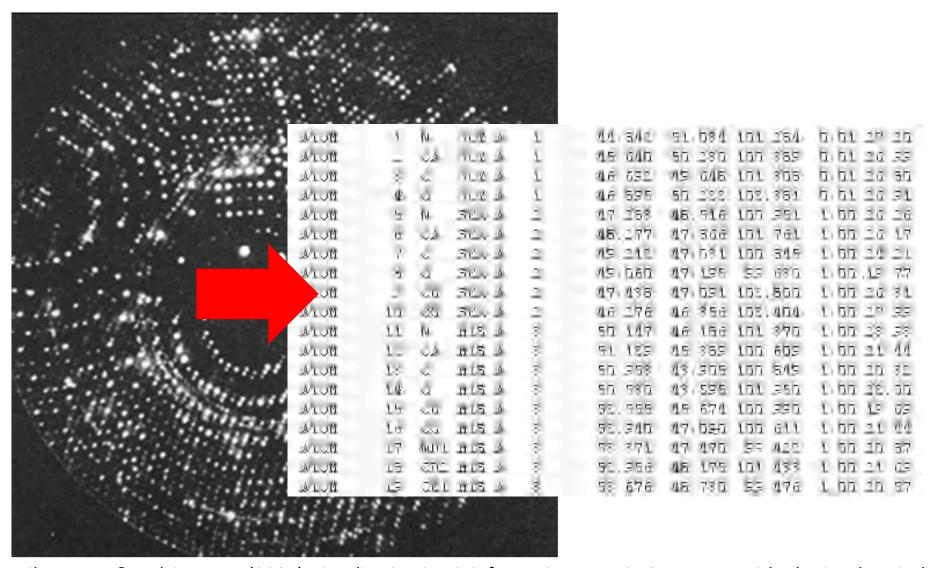
Dali, S. (1931) The persistence of memory



Bagula & Bourke (2012) Klein-Bottle

Our World in Data – Microscopic Structures

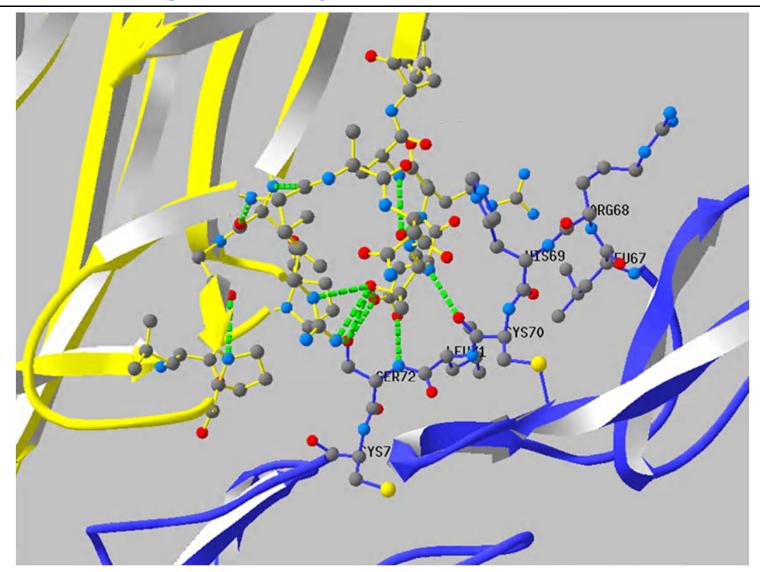




Wiltgen, M. & Holzinger, A. (2005) Visualization in Bioinformatics: Protein Structures with Physicochemical and Biological Annotations. In: *Central European Multimedia and Virtual Reality Conference. Prague, Czech Technical University (CTU), 69-74*

Knowledge Discovery from Data

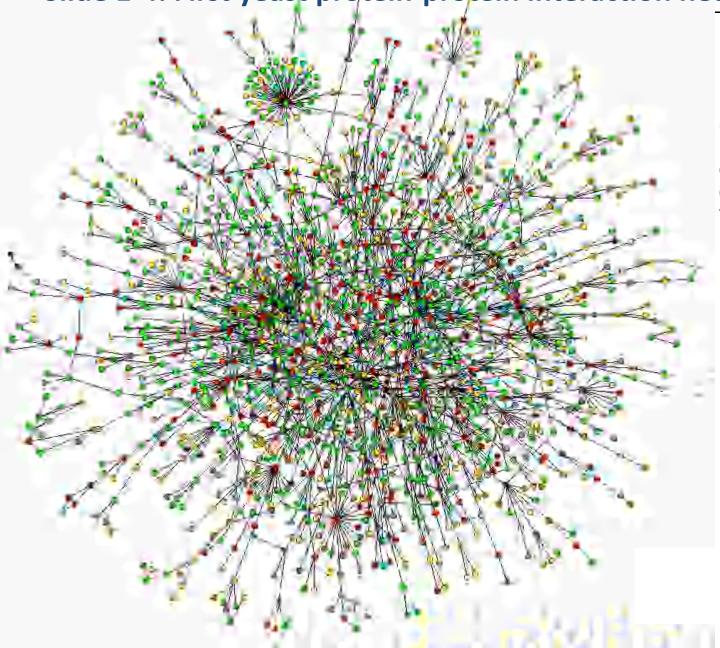




Wiltgen, M., Holzinger, A. & Tilz, G. P. (2007) Interactive Analysis and Visualization of Macromolecular Interfaces Between Proteins. In: *Lecture Notes in Computer Science (LNCS 4799)*. *Berlin, Heidelberg, New York, Springer, 199-212*.

Slide 1-4: First yeast protein-protein interaction network



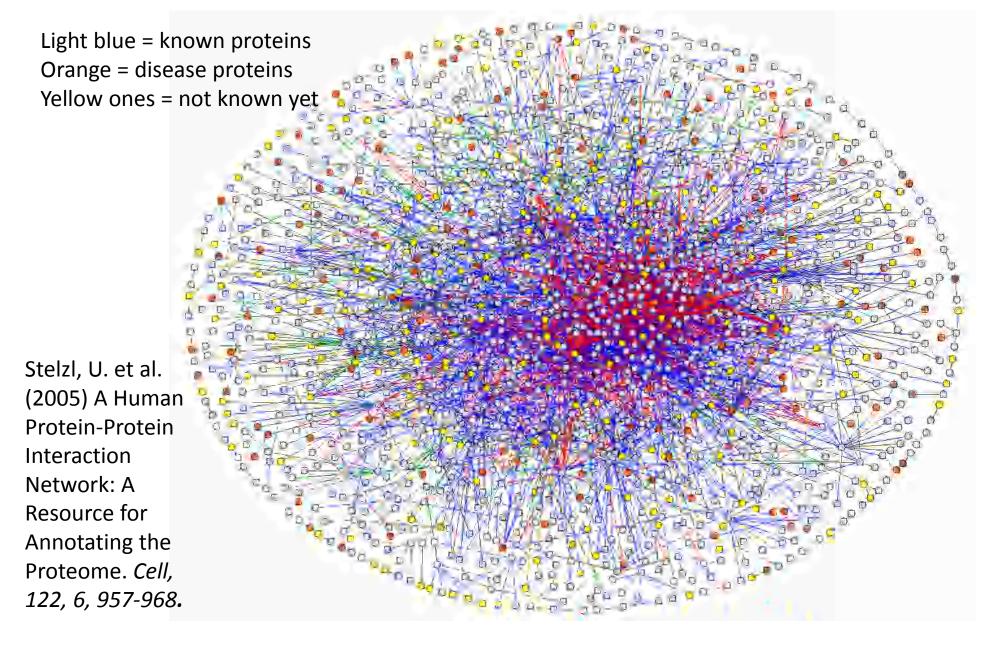


Nodes = proteins
Links = physical interactions
(bindings)
Red Nodes = lethal
Green Nodes = non-lethal
Orange = slow growth
Yellow = not known

Jeong, H., Mason, S. P., Barabasi, A. L. & Oltvai, Z. N. (2001) Lethality and centrality in protein networks. *Nature*, 411, 6833, 41-42.

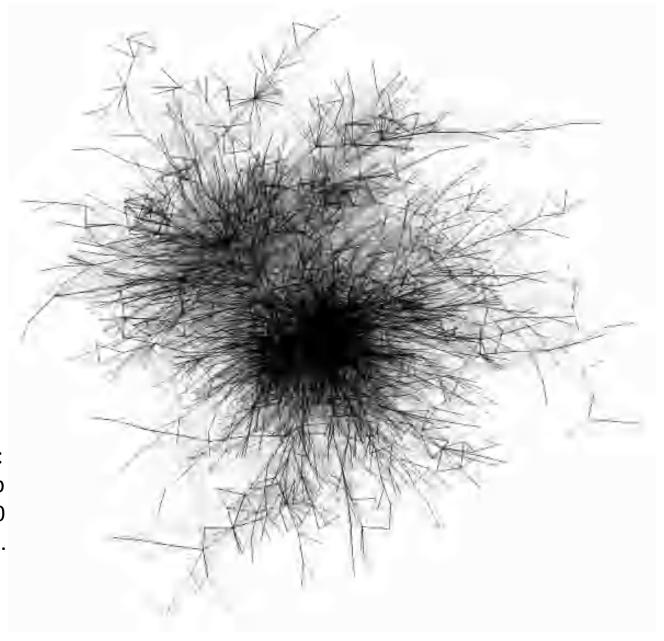
First human protein-protein interaction network





Non-Natural Network Example: Blogosphere

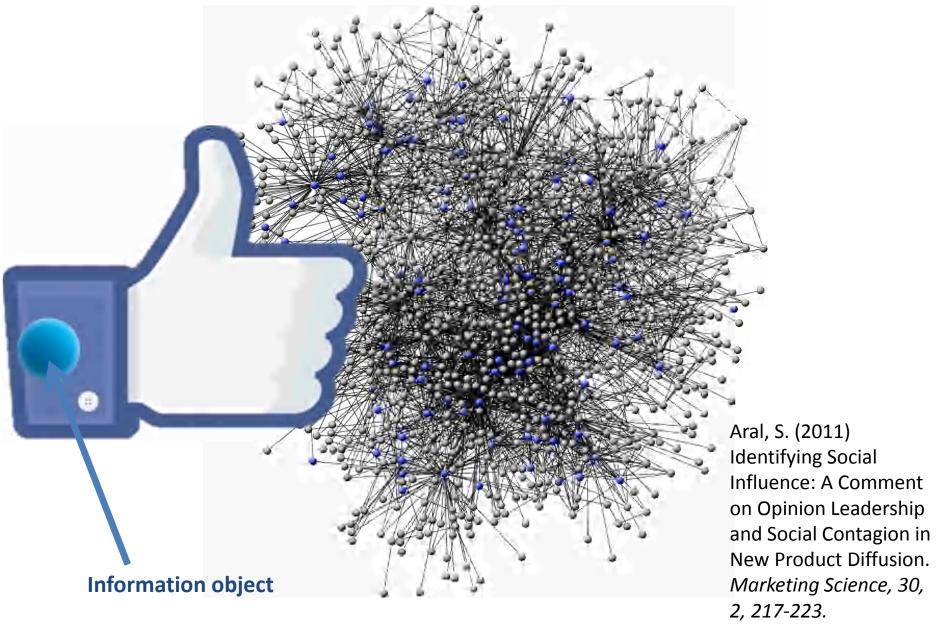




Hurst, M. (2007), Data Mining: Text Mining, Visualization and Social Media. Online available: http://datamining.typep ad.com/data_mining/20 07/01/the_blogosphere. html, last access: 2011-09-24

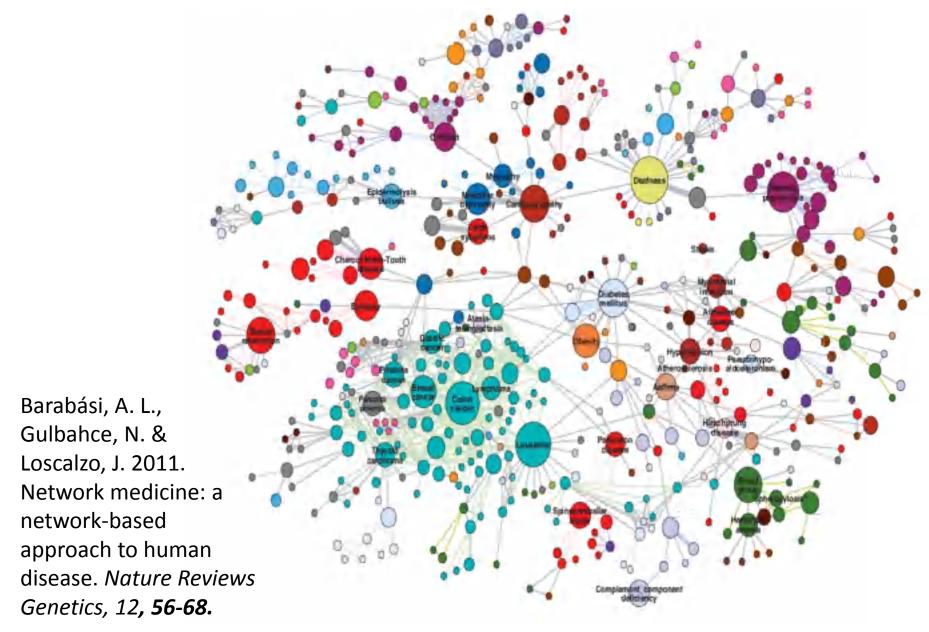
Social Behavior Contagion Network





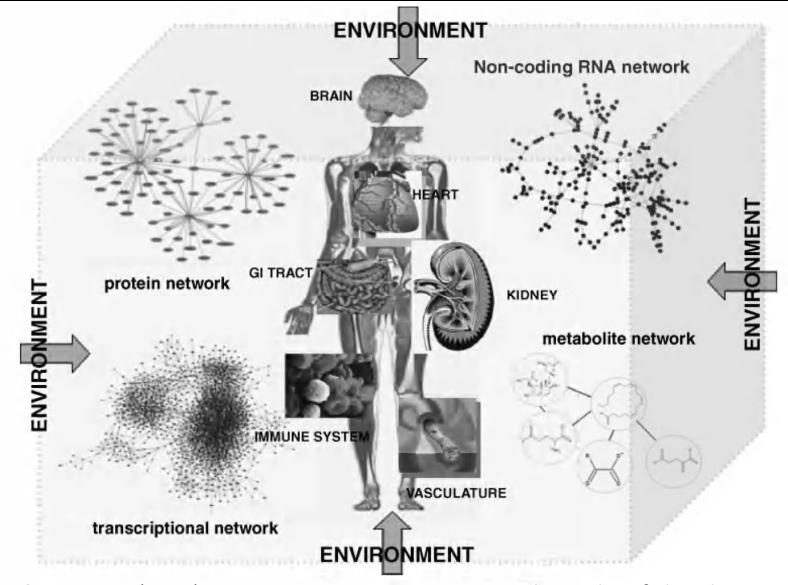
Human Disease Network -> Network Medicine





Identifying Networks in Disease Research





Schadt, E. E. & Lum, P. Y. (2006) Reverse engineering gene networks to identify key drivers of complex disease phenotypes. *Journal of lipid research*, 47, 12, 2601-2613.

Conclusion: Five decades of Health Informatics



- 1960+ Medical Informatics (Early "AI")
 - Focus on data acquisition, storage, accounting (typ. "EDV"), Expert Systems
 - The term was first used in 1968 and the first course was set up 1978!
- 1985+ Health Telematics (Al winter)
 - Health care networks, Telemedicine, CPOE-Systems, ...
- 1995+ Web Era (Al is "forgotten")
 - Web based applications, Services, EPR, distributed systems, ...
- 2005+ Success statistical learning (Al renaissance)
 - Pervasive, ubiquitous Computing, Internet of things, ...
- 2010+ Data Era Big Data (super for AI)
 - Massive increase of data data integration, mapping, ...
- 2020+ Information Era (towards explainable AI)
 - Sensemaking, disentangling the underlying concepts, causality, ...







Exam Questions



Appendix

04

d ... data

h ... hypotheses

$$\mathcal{H}$$
 ... $\{H_1, H_2, ..., H_n\}$ $\forall h, d$...

Likelihood Prior Probability

$$p(h|d) = \frac{p(d|h) * p(h)}{\sum_{h \in H} p(d|h) p(h)}$$

Posterior Probability

Problem in $\mathbb{R}^n o$ complex

P(h): prior belief (probability of hypothesis h before seeing any data)

 $P(d \mid h)$: likelihood (probability of the data if the hypothesis h is true)

 $P(d) = \sum_{h} P(d \mid h)P(h)$: data evidence (marginal probability of the data)

 $P(h \mid d)$: posterior (probability of hypothesis h after having seen the data d)



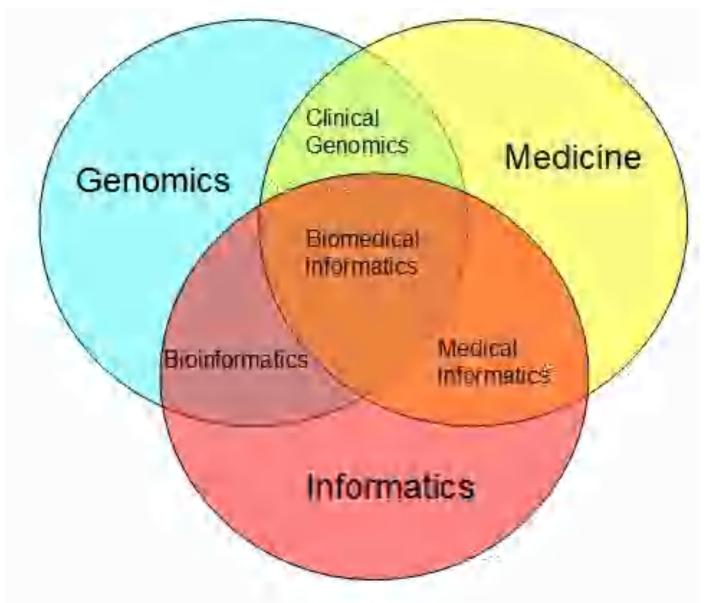


Biomedical informatics (BMI) is the interdisciplinary field that studies and pursues the effective use of biomedical data, information, and knowledge for scientific problem solving, and decision making, motivated by efforts to improve human health

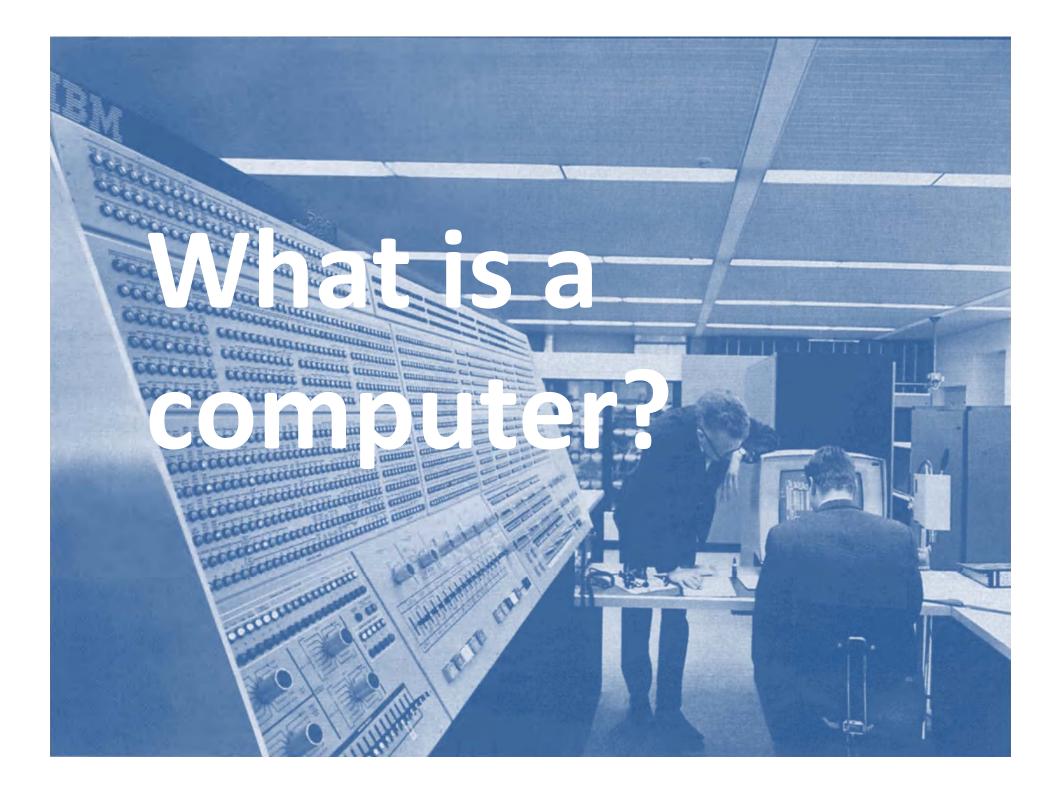
Shortliffe, E. H. (2011). Biomedical Informatics: Defining the Science and its Role in Health Professional Education. In A. Holzinger & K.-M. Simonic (Eds.), *Information Quality in e-Health. Lecture Notes in Computer Science LNCS 7058 (pp. 711-714)*. Heidelberg, New York: Springer.

Computational Sciences meet Life Sciences



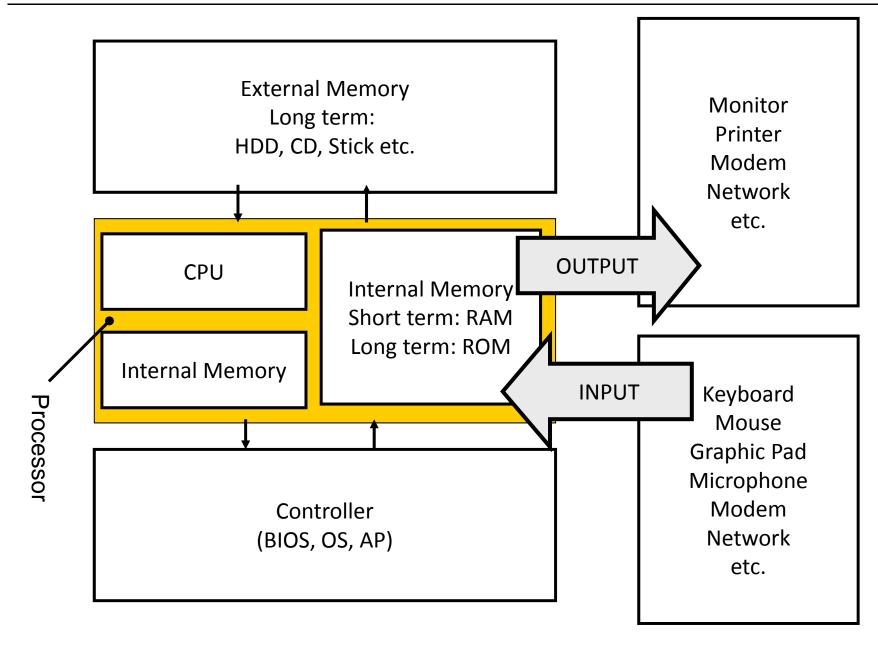


http://www.bioinformaticslaboratory.nl/twiki/bin/view/BioLab/EducationMIK1-2



Computer: Von-Neumann Architecture

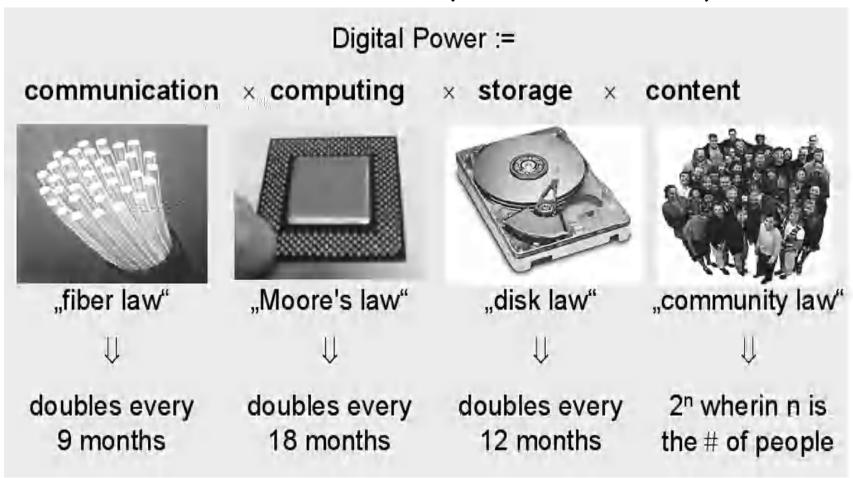




Technological Performance / Digital Power



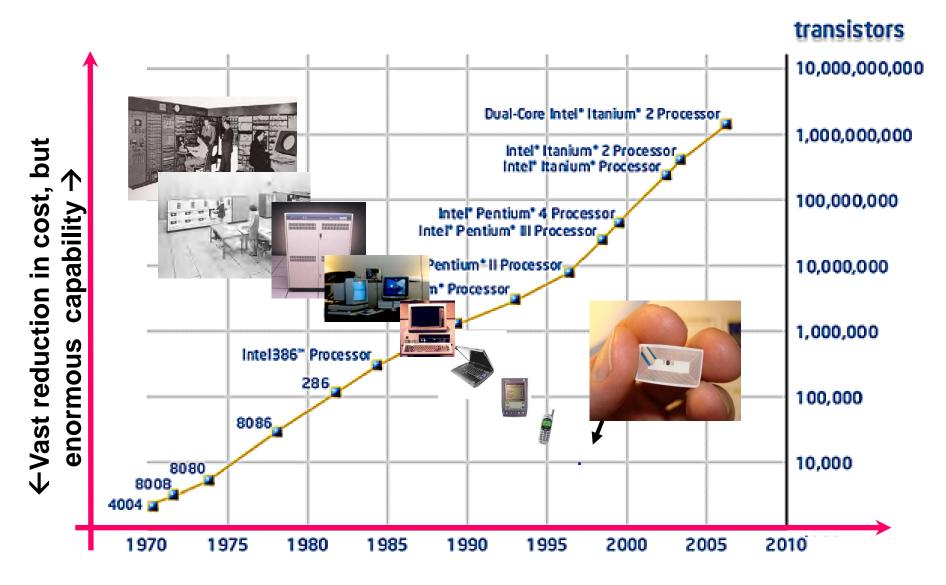
Gordon E. Moore (1965, 1989, 1997)



Holzinger, A. 2002. Basiswissen IT/Informatik Band 1: Informationstechnik. Das Basiswissen für die Informationsgesellschaft des 21. Jahrhunderts, Wuerzburg, Vogel Buchverlag.

Computer cost/size versus Performance

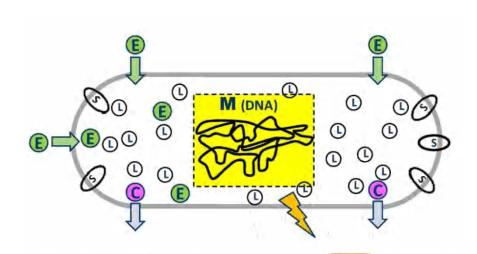




Cf. with Moore (1965), Holzinger (2002), Scholtz & Consolvo (2004), Intel (2007)

Beyond Moore's Law -> biological computing





Memory: 10^7 bit

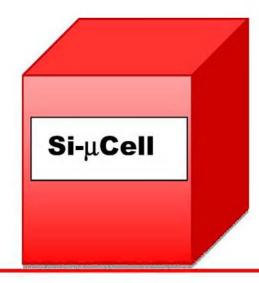
Logic: $>10^6$ bit

Power: 10⁻¹³ W

Heat: $10^{-6} \, \text{W/cm}^2$

Energy/task*: 10⁻¹⁰ J

Task time*: 2400s=40min



Memory: $\sim 10^4$ bit

Logic: ~300–150,000 bit

Power: $\sim 10^{-7} \text{ W}$ Heat: $\sim 1 \text{ W/cm}^2$

Energy/task*: ~10⁻² J

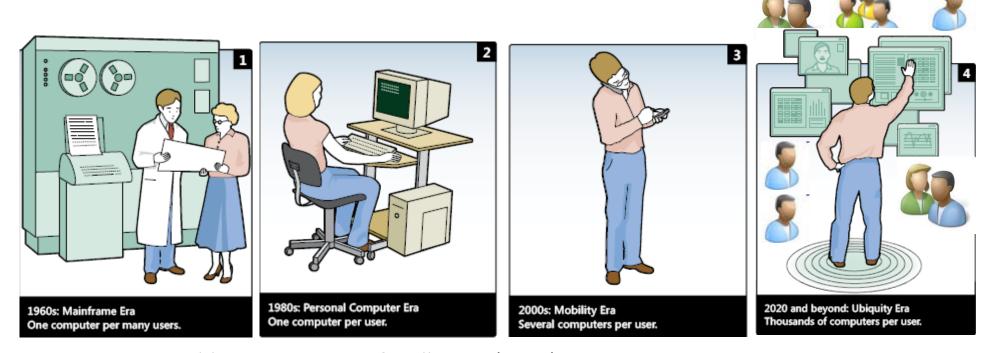
Task time*: $510,000 \text{ s} \sim 6 \text{ days}$

*Equivalent to 10¹¹ output bits

Cavin, R., Lugli, P. & Zhirnov, V. 2012. Science and Engineering Beyond Moore's Law. *Proc. of the IEEE, 100, 1720-49* (L=Logic-Protein; S=Sensor-Protein; C=Signaling-Molecule, E=Glucose-Energy)



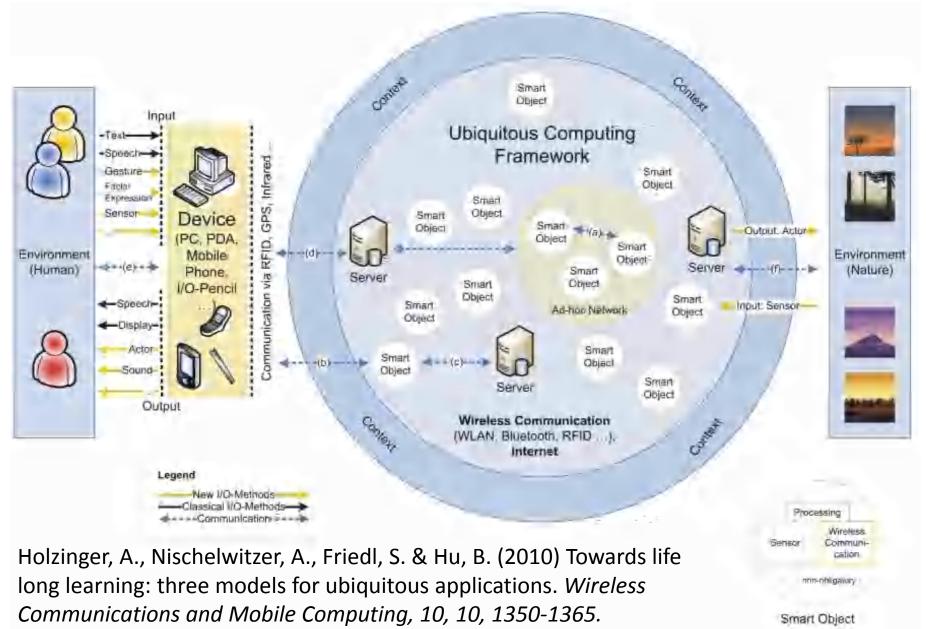
 using technology to augment human capabilities for structuring, retrieving and managing information



Harper, R., Rodden, T., Rogers, Y. & Sellen, A. (2008) Being Human: Human-Computer Interaction in the Year 2020. Cambridge, Microsoft Research.

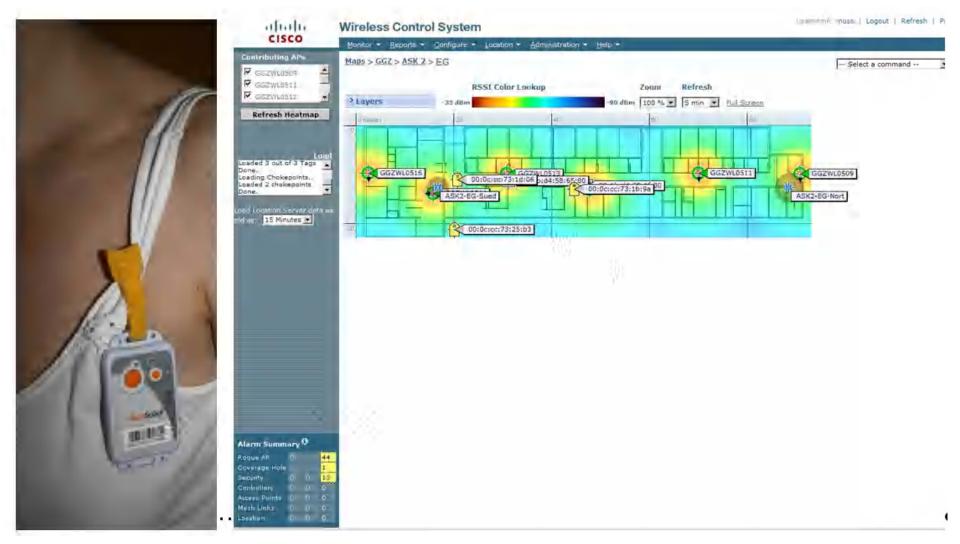
Ubiquitous Computing – Smart Objects





Slide 1-34 Example: Pervasive Health Computing

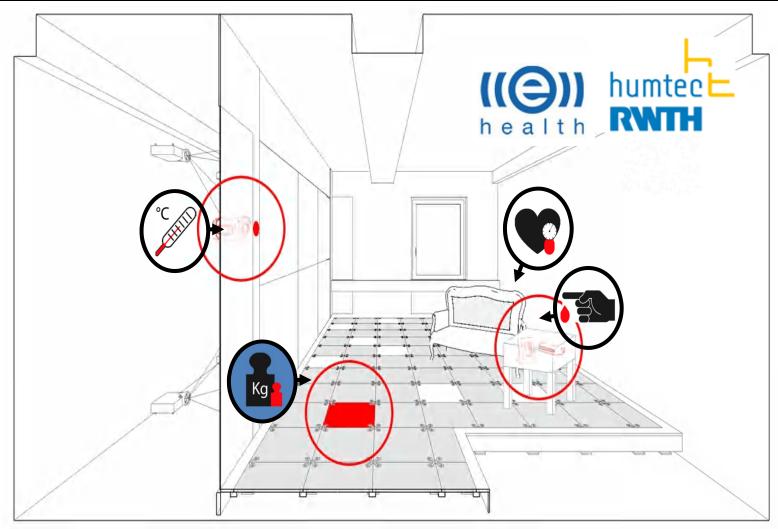




Holzinger, A., Schaupp, K. & Eder-Halbedl, W. (2008) An Investigation on Acceptance of Ubiquitous Devices for the Elderly in an Geriatric Hospital Environment: using the Example of Person Tracking In: *Lecture Notes in Computer Science (LNCS 5105)*. *Heidelberg, Springer, 22-29*.

Ambient Assisted Living - pHealth

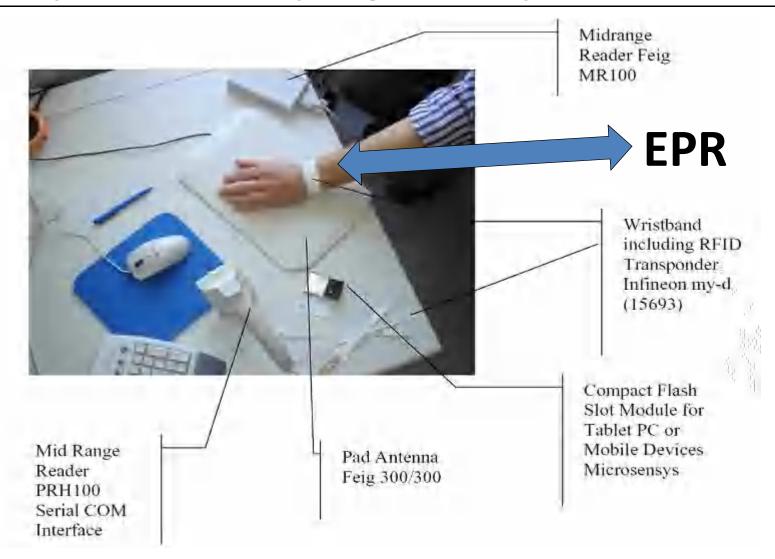




Alagoez, F., Valdez, A. C., Wilkowska, W., Ziefle, M., Dorner, S. & Holzinger, A. (2010) From cloud computing to mobile Internet, from user focus to culture and hedonism: The crucible of mobile health care and Wellness applications. *5th International Conference on Pervasive Computing and Applications (ICPCA)*. *IEEE, 38-45*.

Example Pervasive Computing in the Hospital





Holzinger, A., Schwaberger, K. & Weitlaner, M. (2005) Ubiquitous Computing for Hospital Applications: RFID-Applications to enable research in Real-Life environments 29th Annual IEEE International Computer Software & Applications Conference (IEEE COMPSAC), 19-20.

Smart Objects in the pathology







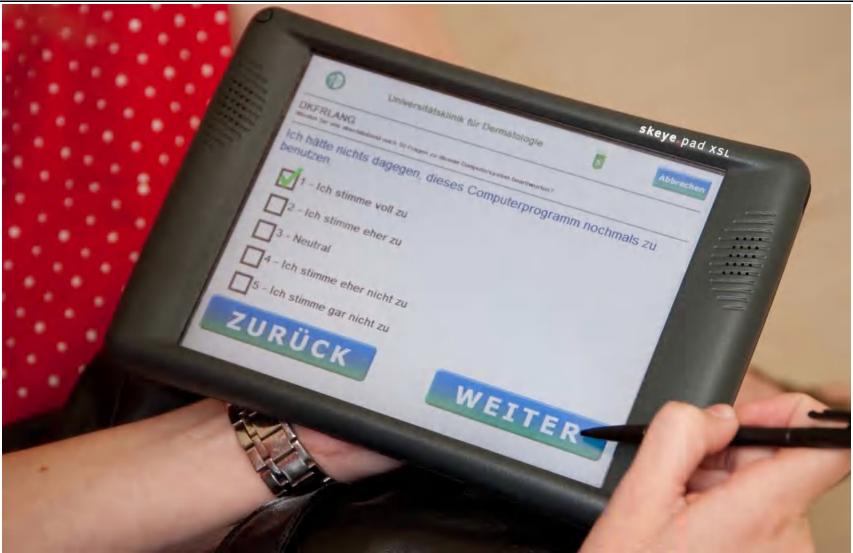




Holzinger et al. (2005)

The medical world is mobile (Mocomed)

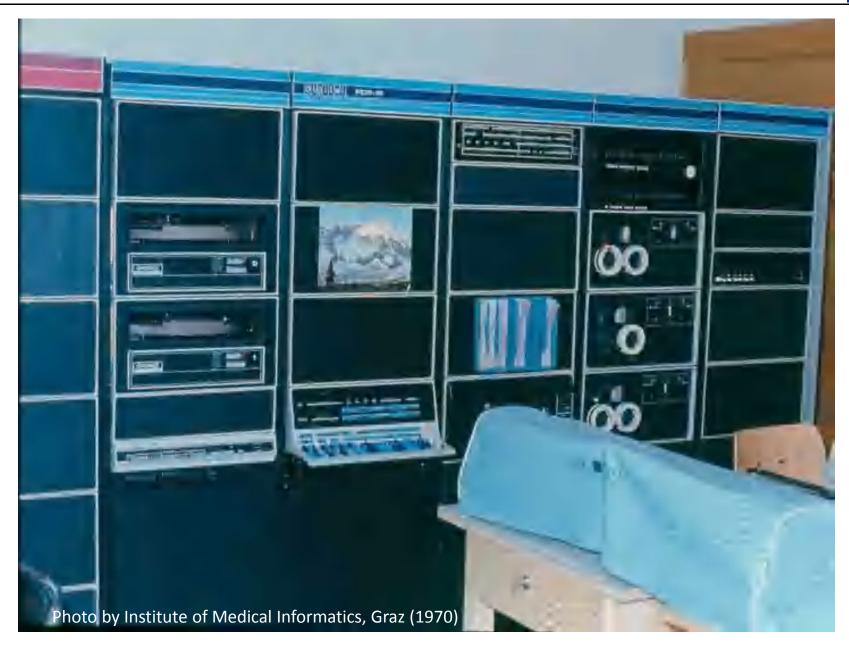




Holzinger, A., Kosec, P., Schwantzer, G., Debevc, M., Hofmann-Wellenhof, R. & Frühauf, J. 2011. Design and Development of a Mobile Computer Application to Reengineer Workflows in the Hospital and the Methodology to evaluate its Effectiveness. *Journal of Biomedical Informatics, 44, 968-977.*

1970 Turning Knowledge into Data



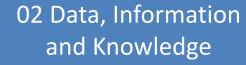




Primer on Probability & Information

Day 1 - Fundamentals

01 Information Sciences meets Life Sciences



03 Decision Making and Decision Support

04 From Expert Systems to Explainable AI









