Welcome to Machine Learning 2013!!



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"Machine learning is about learning, reasoning and acting based on data."

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Outline lecture 1

3(40)

- 1. Introduction and some motivating examples
- 2. Course administration
- 3. Probability distributions and some basic ideas
 - 1. Exponential family
 - 2. Properties of the multivariate Gaussian
 - 3. Maximum Likelihood (ML) estimation
 - 4. Bayesian modeling
 - 5. Robust statistics ("heavy tails")
 - 6. Mixture of Gaussians

Problem classes

4(40)

- Supervised learning. The training data consists of both input and output (target) data.
 - Classification: Discrete output variables.
 - Regression: Continuous output variables.
- **Unsupervised learning.** The training data consists of input data only.
 - Clustering: Discover groups of similar examples in data.
- Reinforcement learning. Finding suitable actions (control signals) in a given situation in order to maximize a reward. Close to control theory.

This course is focused on supervised learning.



- · Learning good controllers for tasks demonstrated by a human expert. Currently a hot topic in many areas (related to ILC).
- Includes learning a model, estimating the states, learning a controller

Pieter Abbeel, Adam Coates and Andrew Y. Ng. Autonomous helicopter aerobatics through apprenticeship learning, International Journal of Robotics Research (IJRR), 29(13):1608-1639, November 2010,

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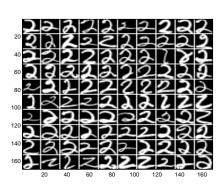
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• Input data: 16 × 16 grayscale images.

- · Task: classify each input image as accurately as possible.
- · This data set will be used throughout the course.
- · Solutions and their performance are summarized on yann.lecun.com/ exdb/mnist/



Data set available from

www-stat.stanford.edu/~tibs/ElemStatLearn/

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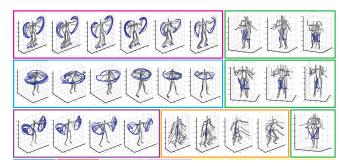
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Example 3 – BNP for dynamical systems

BNP (lecture 11) offers flexible models capable of dealing with

- How many states should be used?
- How many modes? (i.e., hybrid systems)
- What if new modes/states arise over time?



E.B. Fox, E.B. Sudderth, M.I. Jordan, A.S. Willsky. Sharing Features among Dynamical Systems with Beta Processes, Proceeding of Neural Information Processing Systems (NIPS), Vancouver, Canada December 2009.

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Example 4 – animal detection and tracking (I/II)

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Volvo förnyar system som ser faror i mörker

för upptäckt av gående som riskerar att bli påkörda till att också fungera i mörker och för stora djur

Jag möter Volvos tekniker i den tidiga skymningen i ett hägn dan. med ett 30-tal älgar, dov- och vägs kronhjortar. I en Volvo V70 har Kameran är kopplad till en persondator inuti bilen.

Under körning längs vägen vinklar. Både i rörelse och stilla- och ouppmärksamma. stående. fastän bilen kommer
Det är det första fältprovet ANDREAS EIDEHALL sägerattnackmed påslaget halvljus.

ljussignaler varna föraren. Om denne inte ingriper är det tänkt

- Där det finns risk för att förare och passagerare skadas, svarar Andreas Eidehall. som inte bara i Sveriee, utan imånsa bort.

Han förkla

- Systemet, som ännu inte har i hägnet läser datorn i bilen in de olika djuren från olika na förare som är distraherade

i en utveckling som ska leda till att bilen själv lär sig känna igen att fara for att viltkollision devingar föraren att splittar sån der skaren att splittar sån hotar. Den ska då med ljud- och uppmärksamhet mellan vind- röda ljuset på gott håll avslöjar

att bilen bromsar för att undannet i takt med att solen siunker tittar ut genom vindrutan. i väst. Och allt svårare att upp-fatta djuren som lockas till känna igen djuren, säger Anvägen med utlagt foder.

är säkerhetsexpert med djur-detektion som specialitet hos I vårt eget land skedde i fjol

inte har fått något namn, är tänkt att varna förare som är distraherade och

ouppmärksamma. Andreas Etdehall sakerhetsevner

40 000 viltolyckor, berättar han. Av dessa olyckor var 13 procent med älg.

När klockan har blivit 22.30 är det svårt att urskilja djuren som helt oblygt beträder vägen

rutan och bildskärmen. djuren i mörkret fastän jag
Det blir allt skummare i hägknappt kan skönja dessa när jag

dreas Eidehall som tror att den Andreas Eidehall berättar att kommersiella lanseringen i Vol



Automatskydd mot påkörning

Dagens system "pede strian detection with full auto brake" känner igen gående och cyklande i dagslius, var-

det behövs för att undvika en upptäcka stora vilda djur på ■ Med kombinationen radar och infraröd kamera upptäcks

både människor och stora djur ■ Tanken är att täcka en 45 grader stor sektor framför

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Example 4 - animal detection and tracking (II/II)

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- Learning detectors for animals. boosting (lecture 8) promising technology for this.
- Sensor fusion between radar and infrared camera.

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Field of machine learning

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Top 3 conferences on general machine learning

- 1. Neural Information Processing Systems (NIPS)
- 2. International Conference on Machine Learning (ICML)
- 3. European Conference on Machine Learning (ECML) and Inter. Conf. on Artificial Intelligence and Statistics (AISTATS)

Top 3 journals on general machine learning

- 1. Journal of Machine Learning Research (JMLR)
- 2. IEEE Trans. Pattern Analysis and Machine Intelligence (PAMI)
- 3. IEEE Trans. on Neural Networks (TNN)

For new (and non-peer reviewed) material see arXiv.org arxiv.org/list/stat.ML/recent

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• Lecturers: Thomas Schön and Fredrik Lindsten

• Examiner: Thomas Schön

Course administration

- 11 lectures (do not cover everything)
- We will try to provide examples of active research throughout the lectures (especially connections to "our" areas)
- Suggested exercises are provided for each lecture
- Written exam, 3 days (72 hours). Code of honor applies as usual
- All course information, including lecture material is available from the course home page

www.control.isy.liu.se/student/graduate/MachineLearning/

Course administration - projects (3 hp)

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- Voluntary and must be based on a data set.
- Project ideas: discuss with me for ideas or even better, make up your own!!
- Form teams (2-3 students/project).
- Project time line:

Date	Action	
Mar. 20	Project proposals are due	
Mar. 22	Project proposal presentation	
Apr. 19	Final reports are due	
Apr. 24	Final project presentations	

- See course home page for details.
- Note that the deadline for NIPS is in the beginning of June.

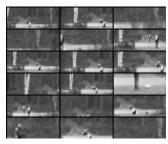
Project example from the 2011 edition

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Detection and classification of cars in video images

Task: Train a detector/classifier, which can be used to detect, track and eventually classify different vehicles in the video recordings.





Positive training samples

Negative training samples

A semi-supervised tracker was also developed (see movie).

Wahlström, N. and Granström, K. Detection and classification of cars in video images, Project report, May, 2011.

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Project example from the dynamic vision course

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Helicopter pose estimation using a map

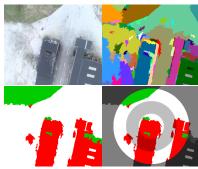




Image from on-board camera (top left), extracted superpixels (top right), superpixels classified as grass, asphalt or house (bottom left) and three circular regions used for computing the class histograms (bottom right).

Fredrik Lindsten, Jonas Callmer, Henrik Ohlsson, David Törnqvist, Thomas B. Schön, Fredrik Gustafsson. **Geo-referencing** for UAV Navigation using Environmental Classification. *Proceedings of the International Conference on Robotics and Automation (ICRA)*, Anchorage, Alaska, USA, May 2010.

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Course overview – Topics

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- 1. Linear regression
- 2. Linear classification
- 3. Expectation Maximization (EM)
- 4. Neural networks
- 5. Gaussian processes (first BNP)
- 6. Support vector machines
- 7. Clustering
- 8. Approximate inference
- 9. Boosting
- 10. Graphical models
- 11. MCMC and sampling methods
- 12. Bayesian nonparametrics (BNP)

Literature

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Course literature:

- 1. Christopher M. Bishop. *Pattern Recognition and Machine Learning*, Springer, 2006.
- Trevor Hastie, Robert Tibshirani and Jerome Friedman. The Elements of Statistical Learning: Data Mining, Inference and Prediction, Second edition, Springer, 2009. (partly)

Recommended side reading:

- Kevin P. Murphy. Machine learning a probabilistic perspective, MIT Press. 2012.
- Daphne Koller and Nir Friedman. Probabilistic Graphical Models Principles and Techniques, MIT Press, 2012.
- David Barber. Bayesian Reasoning and Machine Learning, Cambridge University Press, 2012.



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A few words about probability distributions

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- Important in their own right.
- Forms building blocks for more sophisticated probabilistic models.
- Touch upon some important statistical concepts.

See Chapter 2, Appendix B (useful summary) and Wikipedia.

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The exponential family of distributions over x, parameterized by η ,

$$p(\mathbf{x} \mid \boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^T u(\mathbf{x})\right)$$

Some of the members in the exponential family: Bernoulli, Beta, Binomial, Dirichlet, Gamma, Gaussian, Gaussian-Gamma, Gaussian-Wishart, Student's t, Multinomial, Wishart.

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Multivariate Gaussian (I/VI)

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 $\mathcal{N}(x;\mu,\Sigma) \triangleq \frac{1}{(2\pi)^{n/2}\sqrt{\det\Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$

Let us study a partitioned Gaussian.

$$x = \begin{pmatrix} x_a \\ x_b \end{pmatrix}$$
 $\mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix}$ $\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$

with precision (information) matrix $\Lambda = \Sigma^{-1}$

$$\Lambda = \begin{pmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{pmatrix} = \begin{pmatrix} \Sigma_{aa}^{-1} + \Sigma_{aa}^{-1} \Sigma_{ab} \Delta_a^{-1} \Sigma_{ba} \Sigma_{aa}^{-1} & -\Sigma_{aa}^{-1} \Sigma_{ab} \Delta_a^{-1} \\ -\Delta_a^{-1} \Sigma_{ba} \Sigma_{aa}^{-1} & \Delta_a^{-1} \end{pmatrix}$$

where $\Delta_a = \Sigma_{bb} - \Sigma_{ba} \Sigma_{aa}^{-1} \Sigma_{ab}$ is the Schur complement of Σ_{aa} in Σ .

Multivariate Gaussian (II/VI)

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Theorem (Conditioning)

Let x be Gaussian distributed and partitioned $x = \begin{pmatrix} x_a & x_b \end{pmatrix}^T$, then the conditional density $p(x_a \mid x_b)$ is given by

$$p(x_a \mid x_b) = \mathcal{N}(x_a; \mu_{a|b}, \Sigma_{a|b}),$$

$$\mu_{a|b} = \mu_a + \Sigma_{ab} \Sigma_{bb}^{-1} (x_b - \mu_b),$$

$$\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab} \Sigma_{bb}^{-1} \Sigma_{ba},$$

which using the information (precision) matrix can be written,

$$\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1} \Lambda_{ab} (x_b - \mu_b),$$

 $\Sigma_{a|b} = \Lambda_{aa}^{-1}.$

Multivariate Gaussian (III/VI)

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Multivariate Gaussian (IV/VI)

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Theorem (Marginalization)

Let x be Gaussian distributed and partitioned $x = \begin{pmatrix} x_a & x_b \end{pmatrix}^T$, then the marginal density $p(x_a)$ is given by

$$p(x_a) = \mathcal{N}(x_a; \mu_a, \Sigma_{aa}).$$

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Theorem (Affine transformations)

Assume that x_a , as well as x_b conditioned on x_a , are Gaussian distributed

$$p(x_a) = \mathcal{N}(x_a; \mu_a, \Sigma_a),$$

$$p(x_b \mid x_a) = \mathcal{N}(x_b; Mx_a + b, \Sigma_{b|a}),$$

where M is a matrix and b is a constant vector. The marginal density of x_b is then given by

$$p(x_b) = \mathcal{N}(x_b; \mu_b, \Sigma_b),$$

 $\mu_b = M\mu_a + b,$
 $\Sigma_b = \Sigma_{b|a} + M\Sigma_a M^T.$

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Multivariate Gaussian (V/VI)

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Theorem (Affine transformations, cont.)

The conditional density of x_a given x_b is

$$p(x_a \mid x_b) = \mathcal{N}(x_a; \mu_{a|b}, \Sigma_{a|b}),$$

with

$$\mu_{a|b} = \Sigma_{a|b} \left(M^{T} \Sigma_{b|a}^{-1} (x_{b} - b) + \Sigma_{a}^{-1} \mu_{a} \right)$$

$$= \mu_{a} + \Sigma_{a} M^{T} \Sigma_{b}^{-1} (x_{b} - b - M \mu_{a}),$$

$$\Sigma_{a|b} = \left(\Sigma_{a}^{-1} + M^{T} \Sigma_{b|a}^{-1} M \right)^{-1}$$

$$= \Sigma_{a} - \Sigma_{a} M^{T} \Sigma_{b}^{-1} M \Sigma_{a}.$$

Multivariate Gaussian (VI/VI)

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Multivariate Gaussian's are important building blocks in more sophisticated models.

For more details, proofs and an example where the Kalman filter is derived using the above theorems is provided,

www.control.isy.liu.se/student/graduate/Machine Learning/manip Gauss.pdf

Maximum Likelihood (ML) estimation

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Maximum likelihood provides a systematic way of computing **point estimates** of the unknown parameters θ in a given model, by exploiting the information present in the measurements $\{x_n\}_{n=1}^N$.

Computing ML estimates of the parameters in a model amounts to:

- 1. Model the obtained measurements x_1, \ldots, x_N as a realisation from the stochastic variables $\mathbf{x}_1, \ldots, \mathbf{x}_N$.
- 2. Decide on which model to use.
- 3. Assume that the stochastic variables x_1, \ldots, x_N are conditionally iid.

In ML the parameters θ are chosen in such a way that the measurements $\{x_n\}_{n=1}^N$ are as likely as possible, i.e.,

$$\widehat{\theta}^{\mathsf{ML}} = \underset{\theta}{\operatorname{arg\,max}} \ p(x_1, \cdots, x_N \mid \theta).$$

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Bayesian modeling

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The **goal** in Bayesian modeling is to compute the posterior $p(\theta \mid x_{1:N})$.

Provided that it makes sense from a modeling point of view it is convenient to choose prior distributions rendering a computationally tractable posterior distribution.

This leads to the so called **conjugate priors** (if the prior and the posterior have the same functional form, the prior is said to be a conjugate prior for the likelihood).

Again, only make use of conjugate priors if this makes sense from a modeling point of view!

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Conjugate priors – example 1 (I/II)

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Let $X = \{x_n\}_{n=1}^N$ be independent identically distributed (iid) observations of $x \sim \mathcal{N}(\mu, \sigma^2)$. Assume that the variance σ^2 is known.

The likelihood is given by

$$p(X \mid \mu) = \prod_{n=1}^{N} p(x_n \mid \mu) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2\right)$$

If we choose the prior as $p(\mu) = \mathcal{N}(\mu \mid \mu_0, \sigma_0^2)$, the posterior will also be Gaussian. Hence, this Gaussian prior is a conjugate prior for the likelihood.

Conjugate priors – example 1 (II/II)

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The resulting posterior is

$$p(\mu \mid X) = \mathcal{N}(\mu_B, \sigma_B^2),$$

where the parameters are given by

$$\mu_B=rac{\sigma^2}{N\sigma_0^2+\sigma^2}\mu_0+rac{N\sigma_0^2}{N\sigma_0^2+\sigma^2}\mu_{ extsf{ML}}, \ rac{1}{\sigma_B^2}=rac{1}{\sigma_0^2}+rac{N}{\sigma^2}.$$

The ML estimate of the mean is

$$\mu_{\mathsf{ML}} = \frac{1}{N} \sum_{n=1}^{N} x_n.$$

Conjugate priors – some examples

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Likelihood	Model Parameters	Conjugate Prior
Normal (known mean)	Variance	Inverse-Gamma
Multivariate Normal	Precision	Wishart
(known mean)		
Multivariate Normal	Covariance	Inverse-Wishart
(known mean)		
Multivariate Normal	Mean and covariance	Normal-Inverse-
		Wishart
Multivariate Normal	Mean and precision	Normal-Wishart
Exponential	Rate	Gamma

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Conjugate prior is just one of many possibilities!

Note that using a conjugate prior is **just one** of the many possible choices for modeling the prior! If it makes sense, use it, since it leads to simple calculations.

Let's have a look at an example where we do not make use of the conjugate prior and end up in a useful and interesting result.

Linear regression models the relationship between a continuous target variable t and an (input) variable x according to

$$t_n = w_0 + w_1 x_{1,n} + w_2 x_{2,n} + \dots + w_D x_{D,n} + \epsilon_n$$

= $w^T \phi(x_n) + \epsilon_n$,

where
$$\phi(x_n) = \begin{pmatrix} 1 & x_{1,n} & \dots & x_{D,n} \end{pmatrix}^T$$
 and $n = 1,\dots,N$.

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Conjugate prior is just one of many possibilities! 31(40)

Let $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$, resulting in the following likelihood

$$p(t_n \mid w) = \mathcal{N}(t_n \mid w^T \phi(x_n), \sigma^2).$$

Let us now assume w_n to be independent and Laplacian distributed (i.e. not conjugate prior), $w_n \sim \mathcal{L}(0, 2\sigma^2/\lambda)$

Def. (Laplacian distribution) $\mathcal{L}(x \mid a, b) = \frac{1}{2b} \exp\left(-\frac{|x-a|}{b}\right)$.

The resulting MAP estimate is given by,

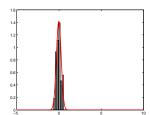
$$w^{\mathsf{MAP}} = rg \max_{w} \ \sum_{n=1}^{N} (t_n - w^T \phi(x_n))^2 + \lambda \sum_{n=1}^{D} |w_n|$$

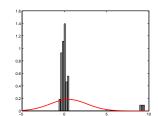
Known as the **LASSO** and it leads to sparse estimates.

Robust statistics

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Modeling the error as a Gaussian leads to very high sensitivity to outliers in the data. This is due to the fact that the Gaussian assigns very low probability to points far from the mean. The Gaussian is said to have "thin tails".





Two possible solutions

- 1. Model using a distribution with "heavy tails".
- 2. Outlier detection models

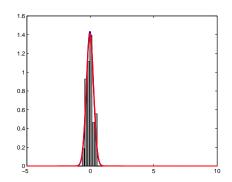
Example: heavy tails (I/III)

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Generate N = 50 samples,

$$x \sim \mathcal{N}(0, 0.1)$$

Plot showing a realization (gray histogram) and the corresponding ML estimate of a Gaussian (red) and a Student's t-distribution (blue).



Note that (as expected?) the red curve sits on top of the blue curve.

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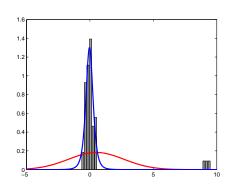


Example: heavy tails (II/III)

Let us now add 3 outliers 9.9.2 and 9.5 to the data set.

Plot showing resulting ML estimate of a Gaussian (red) and a Student's t-distribution (blue).

Clearly the Student's t-distribution is a better model here!



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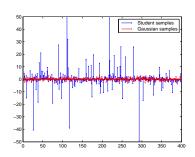
34(40)

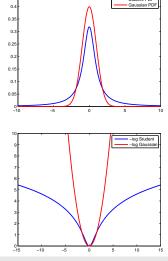
Example: heavy tails (III/III)

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Below: 400 samples from a Student's t-distribution and a Gaussian distribution.

Right: The corresponding pdf's and negative log-likelihoods.





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Outlier detection models

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Model the data as if it comes from a mixture of two Gaussians,

$$p(x_i) = p(x_i | k_i = 0)p(k_i = 0) + p(x_i | k_i = 1)p(k_i = 1)$$

= $\mathcal{N}(0, \sigma^2)p(k_i = 0) + \mathcal{N}(0, \alpha\sigma^2)p(k_i = 1).$

where $\alpha > 1$, $p(k_i = 0)$ is the probability that the sample is OK and $p(k_i = 1)$ is the probability that the sample is an outlier.

Note the similarity between these two "robustifications":

- The Student's t-distribution is an infinite mixture of Gaussians. where the mixing is controlled by the ν -parameter.
- The outlier detection model above consists of a sum of two Gaussians.



Summary – robust statistics

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- Do not use distributions with thin tails (non-robust) if there are outliers present. Use more realistic robust "heavy tailed" distribution such as the Student's t-distribution or simply a mixture of two Gaussians.
- A nice account on robustness in a computer vision context is available in Section 3.1 in

B. Triggs, P. McLauchlan, R. Hartley, and A. Fitzgibbon. **Bundle Adjustment - A Modern Synthesis.** In: *Vision algorithms: theory and practice.* Lecture Notes in Computer Science, Vol 1883:152–177. Springer, Berlin, 2000. dx.doi.org/10.1007/3-540-44480-7_21

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Example - range measurements with outliers

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We measure range (r), contaminated by a disturbance $d_n \geq 0$ and noise $e_n \sim \mathcal{N}(0, \sigma^2)$, $y_n = r + d_n + e_n$. Compute the MAP estimate of $\theta = \{r, d_1, \ldots, d_N\}$ under an exponential prior on d_n ,

$$p(d_n) = \begin{cases} \lambda \exp(-\lambda d_n), & d_n \ge 0, \\ 0, & d_n < 0. \end{cases}$$

Resulting problem

$$\widehat{\theta}^{\mathsf{MAP}} = \argmax_{\theta} p(\theta \mid y_{1:N}) = \arg\min_{\theta} \sum_{n=1}^{N} N \frac{(y_n - r - d_n)^2}{\sigma^2} + \lambda \sum_{n=1}^{N} d_n$$

For details, see Example 2.2. in the PhD thesis of Jeroen Hol.

This principle is used for ultra-wideband positioning, incorporated into MotionGrid (www.xsens.com/en/general/motiongrid) from our partners Xsens (www.xsens.com).

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Important message!

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Given the computational tools that we have today it can be rewarding to resist the Gaussian convenience!!

We will try to repeat and illustrate this message throughout the course using theory and examples.

A few concepts to summarize lecture 1

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Supervised learning: The data consists of both input and output signals (e.g., regressions and classification).

Unsupervised learning: The data consists of output signals only (e.g., clustering).

Reinforcement learning: Finding suitable actions (control signals) in a given situation in order to maximize a reward. (Very similar to control theory)

Conjugate prior: If the posterior distribution is in the same family as the prior distribution, the prior and posterior are *conjugate distributions* and the prior is called a conjugate prior for the likelihood.

Maximum likelihood: Choose the parameters such that the observations are as likely as possible.