

# Non-parametric Bayesian Methods in Machine Learning

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# Outline

- ▶ (My) Bayesian philosophy
- ▶ Gaussian Processes for Regression and Classification (Monday)
  - ▶ GP preliminaries
  - ▶ *Application 1:* typing on touch-screens
  - ▶ Classification (including semi-supervised)
  - ▶ *Application 2:* clinical (dis)-agreement
- ▶ Dirichlet Process flavoured Cluster Models (Tuesday)
  - ▶ DP preliminaries
  - ▶ *Application 3:* Identifying metabolites
  - ▶ *Application 4:* Cluster models for multiple data views
- ▶ Summary

## Relevant publications

- ▶ The four applications are described in the following papers:
  - ▶ Uncertain Text Entry on Mobile Devices Weir et. al, CHI 2014
  - ▶ Investigating the Disagreement Between Clinicians' Ratings of Patients in ICUs Rogers et. al 2013, IEEE Trans Biomed Health Inform
  - ▶ MetAssign: Probabilistic annotation of metabolites from LC–MS data using a Bayesian clustering approach Daly et. al, Bioinformatics, under review
  - ▶ Infinite factorization of multiple non-parametric views Rogers et. al, Machine Learning 2009

# About me

- ▶ I'm not a statistician by training (don't ask me to prove anything!).
- ▶ Education:
  - ▶ Undergraduate Degree: Electrical and Electronic Engineering (Bristol)
  - ▶ PhD: Machine Learning Techniques for Microarray Analysis (Bristol)
- ▶ Currently:
  - ▶ Lecturer: Computing Science
  - ▶ Research Interests: Machine Learning and Applied Statistics in Computational Biology and Human-Computer Interaction (HCI)

# Lecture 3: Application: Touchscreen typing

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# Typing on touchscreens

- ▶ Most people have smartphones
- ▶ Most smartphones have touchscreens
- ▶ Touchscreens are small
- ▶ Keyboards on touchscreens are small
- ▶ Typing on them is hard!
  - ▶ ... but people type on them a lot

## Background 1: Why is it hard?

- ▶ Occlusion of target by finger
- ▶ 'fat finger' problem
- ▶ Small targets
- ▶ Demo: <http://bit.ly/1nBws97>

## Background 1: Why is it hard?

- ▶ Occlusion of target by finger
- ▶ 'fat finger' problem
- ▶ Small targets
- ▶ Demo: <http://bit.ly/1nBws97>
- ▶ Quite a bit of work in this area:
  - ▶ Holz and Baudisch
  - ▶ Henze (100,000,000 taps)
- ▶ Collecting data is fairly easy

## Background 2: All users are different

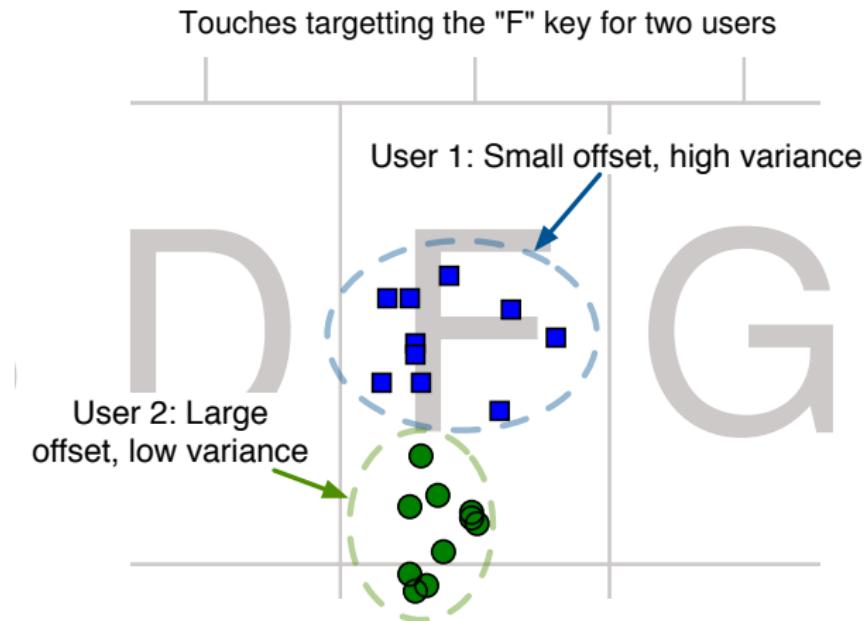


Figure 5 : Touches recorded by two users aiming for the 'F' key. User 2 has high bias and low variance, user 1 has low bias and high variance.

## Background 3: Current systems (maybe?)

- ▶ Touch is boxed into nearest key.
- ▶ Key ID is passed to a Statistical Language Model (SLM).
- ▶ SLM is made up of probabilities of observing certain character strings (from large text corpora).
- ▶ SLM can swap characters to make the character string more likely.
  - ▶ e.g. 'HELLP → HELLO'

# Our idea

- ▶ There is a lot of uncertainty present in touch (bias and variance)
- ▶ Boxing a touch into a key is probably bad
- ▶ Why can't we pass a *distribution* to the SLM?
  - ▶ Pass the uncertainty onwards
  - ▶ Being Bayesian!

## Our idea

- ▶ There is a lot of uncertainty present in touch (bias and variance)
- ▶ Boxing a touch into a key is probably bad
- ▶ Why can't we pass a *distribution* to the SLM?
  - ▶ Pass the uncertainty onwards
  - ▶ Being Bayesian!
- ▶ Can use a user specific GP regression model to predict target from input touch.

## The model

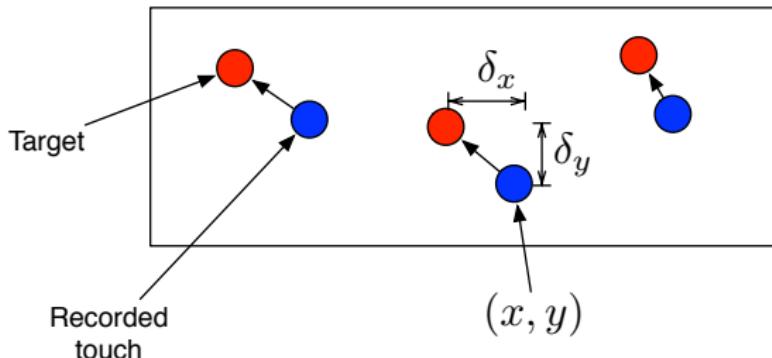
- ▶ We use independent GP regressions for predicting  $x$  and  $y$  offsets.
- ▶ Training data:
  - ▶ Each user typed phrases provided to them.
  - ▶ Data: the  $x, y$  location of the recorded touch (i.e.  $\mathbf{x}_n = [x_n, y_n]^T$ ). Target: the center of the intended key minus the touch (i.e. the offset).

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- ▶ Used a GP with zero mean and a composite covariance:

$$C(\mathbf{x}_1, \mathbf{x}_2) = a\mathbf{x}_1^T \mathbf{x}_2 + (1 - a)\exp\{-\gamma||\mathbf{x}_1 - \mathbf{x}_2||^2\}$$

# The model



$$\delta_x \sim GP(\mathbf{0}, \mathbf{C})$$

$$\delta_y \sim GP(\mathbf{0}, \mathbf{C})$$

$$\mathbf{C}_{nm} = f((x_n, y_n), (x_m, y_m))$$

- ▶  $x$  and  $y$  offsets both depend on  $x$  and  $y$  position of touch
- ▶ Have also used raw capacitive sensor data as input
  - ▶ Potentially better (more info) but only accessible on some devices

## System cartoon



**Figure 6 :** Train GPs to predict the intended touch from an input touch. The flexibility of GPs means that the mean and covariance of the offset can vary across the keyboard.

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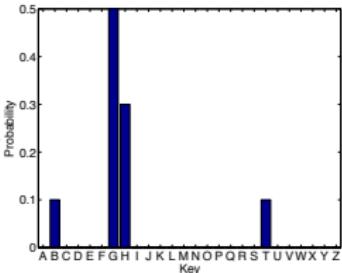


**Figure 6 :** Train GPs to predict the intended touch from an input touch. The flexibility of GPs means that the mean and covariance of the offset can vary across the keyboard.

# System cartoon



Integrate  
predictive  
Gaussian over  
keys to obtain  
distribution



BAB -> BAG

Combine  
probabilities with  
those from  
language model

Figure 7 : The complete system

# Video

- ▶ <http://www.youtube.com/watch?v=1lQI5gV5l74>

## The experiment

- ▶ 10 participants
- ▶ Calibration data collected for each
  - ▶ Note: calibration task matters
- ▶ each did  $3 \times 45$  minute sessions, typing whilst sitting, standing and walking. [more details in paper]
- ▶ Compared:
  - ▶ GPtype (our system), Swiftkey (commercial Android keyboard), GP only (just offset, no SLM), baseline (boxing, no SLM).

# Results

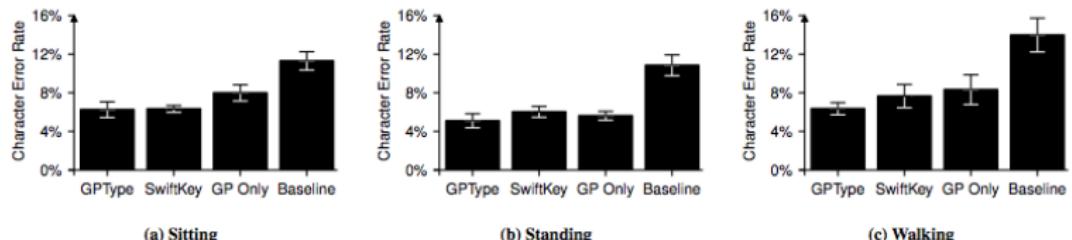


Figure 4. Character error rates for the two keyboards we evaluated, separated by mobility condition (Study 2). Plots show mean and standard error across all participants. The baseline method represents the literal keys touched, while GP Only shows the keys hit after the mean GP offset is applied.

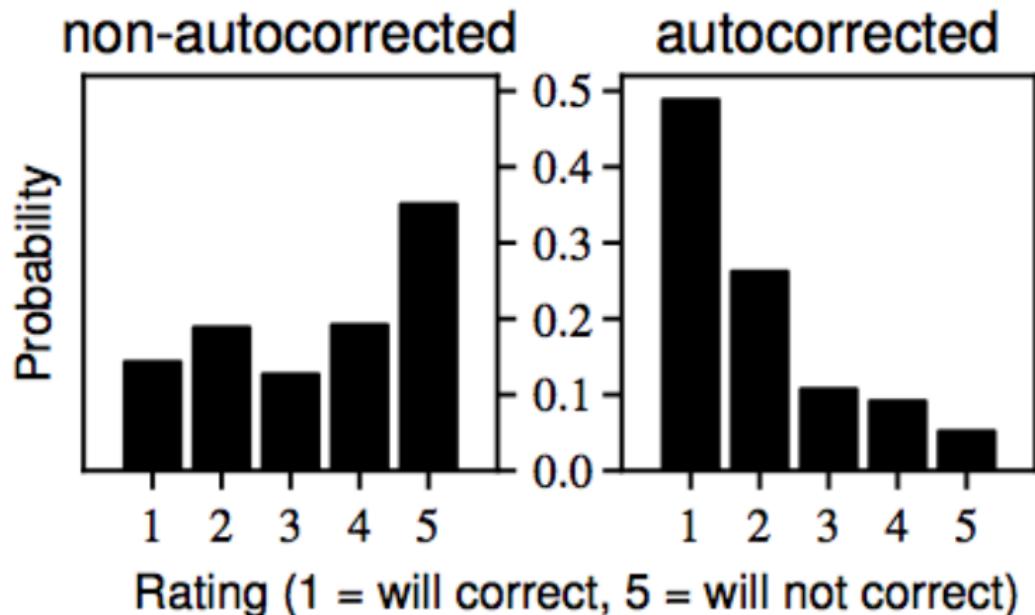
Figure 8 : Results of GPTYPE experiment

- ▶ GPTYPE marginally (stat sig) better than Swiftkey.
  - ▶ A **lot** of people work on SwiftKey
- ▶ Baseline awful!

# Explicit uncertainty control

- ▶ In GPType, uncertainty is handled implicitly
- ▶ As user typing becomes more uncertain, more power given to language model
- ▶ Could users *explicitly* control this?
  - ▶ Certain inputs: no SLM control (slang, names, etc)
  - ▶ Uncertain inputs: high SLM control
- ▶ Use pressure to control certainty:
  - ▶ High pressure: high certainty
  - ▶ Low pressure: low certainty

## Do users know when SLM will fail?



- ▶ Users given phrases and asked whether they thought autocorrect would change them incorrectly
- ▶ Users quite good at understanding SLM failings

# ForceType



- ▶ Modified Synaptics Forcepad
- ▶ Pressure mapped to Gaussian variance (no GP)
- ▶ System explained to users
- ▶ Users type phrases with and without forcetype

# ForceType: Results

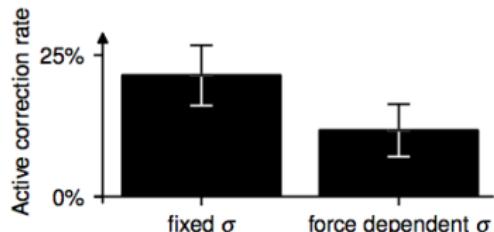


Figure 8. ForceType requires significantly fewer active corrections from users when entering text. Required corrections dropped by  $\approx 10$  percentage points. Errors bars are 1 sd.

- ▶ ForceType reduced number of corrections performed by users (top)
- ▶ ForceType improved overall text entry rate

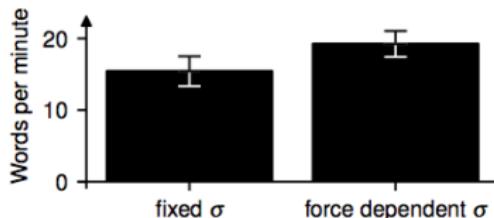


Figure 9. ForceType enabled users to enter phrases > 20% faster. A significant increase over the baseline. Errors bars are 1 sd.

# Conclusions

- ▶ GP regression is key to the approach: we make no parametric assumptions (what would they be?)
- ▶ ... and get probabilistic predictions
- ▶ ... that can be fed to the SLM – (un)certainty is passed to the SLM
- ▶ Performance is promising

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# Conclusions

- ▶ GP regression is key to the approach: we make no parametric assumptions (what would they be?)
- ▶ ... and get probabilistic predictions
- ▶ ... that can be fed to the SLM – (un)certainty is passed to the SLM
- ▶ Performance is promising
- ▶ Can also use pressure to provide explicit uncertainty control
- ▶ More info:
  - ▶ <http://www.youtube.com/watch?v=llQI5gV5l74>
  - ▶ <http://pokristensson.com/pubs/WeirEtAlCHI2014.pdf>
  - ▶ Acknowledgements: Daryl Weir, Per Ola Kristensson, Keith Vertanen, Henning Pohl

# Lecture 4: GPs for classification and ordinal regression via the auxiliary variable trick

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# GPs for Classification and ordinal regression

- ▶ What if our observation model is non-Gaussian?
  - ▶ Classification:

$$P(y_n = 1 | f_n) = \int_{-\infty}^{f_n} \mathcal{N}(z|0, 1) dz = \phi(f_n)$$

- ▶ Logistic Regression:

$$P(y_n = k | f_n) = \phi(b_{k+1}) - \phi(b_k)$$

- ▶ etc

- ▶ Analytical inference is no longer possible
- ▶ I'll cover how to do inference in these models and extensions with the *auxiliary variable trick*

## Binary classification

- ▶ Problem setup: we observe  $N$  data / target pairs  $(\mathbf{x}_n, y_n)$  where  $y_n \in \{0, 1\}$
- ▶ Place a GP prior on a set of latent variables  $f_n$

$$\mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$

- ▶ Use the probit likelihood:

$$P(y_n = 1 | f_n) = \phi(f_n) = \int_{-\infty}^{f_n} \mathcal{N}(z|0, 1) dz$$

- ▶ Inference in this form is hard

# Auxiliary Variable Trick

- ▶ Re-write the probit function:

$$\begin{aligned} P(y_n = 1 | f_n) &= \int_{-\infty}^{f_n} N(z|0, 1) dz \\ &= \int_{-\infty}^0 N(z| -f_n, 1) dz \\ &= \int_0^\infty N(z|f_n, 1) dz \\ &= \int_{-\infty}^\infty \delta(z > 0) \mathcal{N}(z|f_n, 1) dz \end{aligned}$$

where  $\delta(expr)$  is 1 if  $expr$  is true, and 0 otherwise.

## Auxiliary Variable Trick

- If we define  $P(y_n = 1|z_n) = \delta(z_n > 0)$  then we have:

$$P(y_n = 1|f_n) = \int_{-\infty}^{\infty} P(y_n = 1|z_n)p(z_n|f_n) dz_n$$

- and could therefore remove the integral to obtain a model including  $z_n$ :

$$p(y_n = 1, z_n | f_n) = P(y_n = 1|z_n)p(z_n|f_n)$$

- Doing inference in this model (i.e. with additional variables  $z_n$ ) is much easier (but still not analytically tractable)
- Note:  $P(y_n = 0|z_n) = \delta(z_n < 0)$

## Example - Gibbs sampling for binary classification

- ▶ An easy way to perform inference in the augmented model is via Gibbs sampling
- ▶ Sample  $z_n|f_n, y_n$ :

$$p(z_n|f_n, y_n = 0) \propto \delta(z_n < 0)\mathcal{N}(z_n|f_n, 1)$$

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- ▶ Sample  $\mathbf{f}|\mathbf{z}, \mathbf{C}$

$$p(\mathbf{f}|\mathbf{z}, \mathbf{C}) = \mathcal{N}(\boldsymbol{\mu}_f, \boldsymbol{\Sigma}_f)$$

where

$$\boldsymbol{\Sigma}_f = (\mathbf{I} + \mathbf{C}^{-1})^{-1}, \quad \boldsymbol{\mu}_f = \boldsymbol{\Sigma}_f^{-1}\mathbf{z}$$

- ▶ Repeat ad infinitum

## Example - Gibbs sampling for binary classification

- ▶ To make predictions:
  - ▶ At each sampling step, do a (noise-free) GP regression using the current sample of  $\mathbf{f}$  to get a density over  $f_*$  (Details in a previous slide).
  - ▶ Sample a specific realisation of  $f_*$  from this density.
  - ▶ Compute  $\phi(f_*)$  (or sample a  $z_*$  and then record whether it's  $> 0$  or not)
  - ▶ Average this value over all Gibbs sampling iterations!

## Example - binary classification

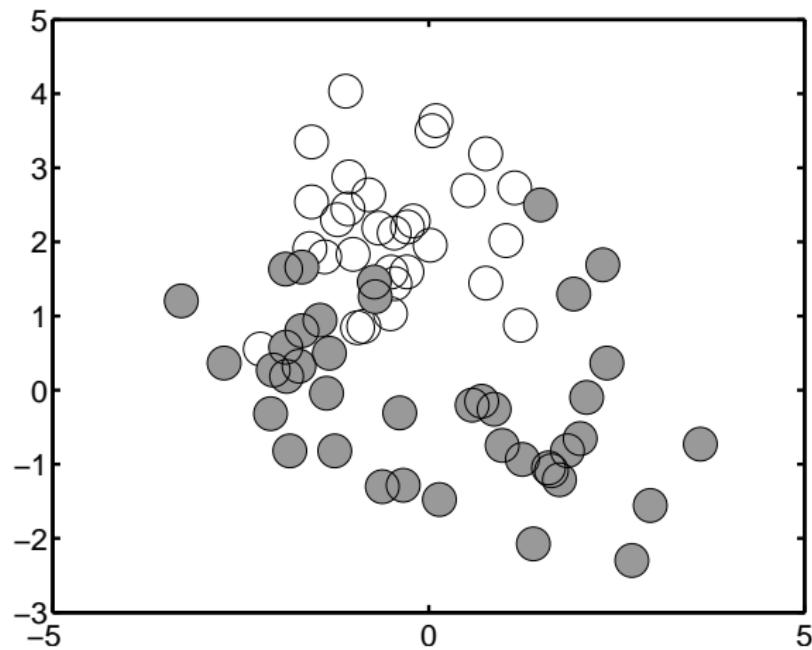


Figure 9 : Some simple classification data

## Example - binary classification

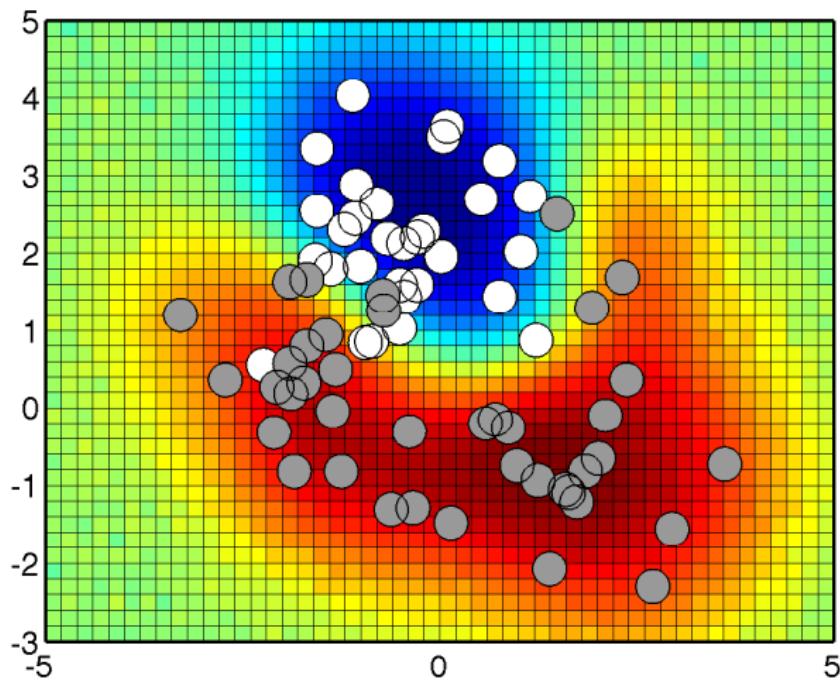


Figure 10 : Predictive probabilities averaged over 1000 Gibbs samples using an RBF covariance. As  $\gamma$  is increased, the model overfits.

## Example - binary classification

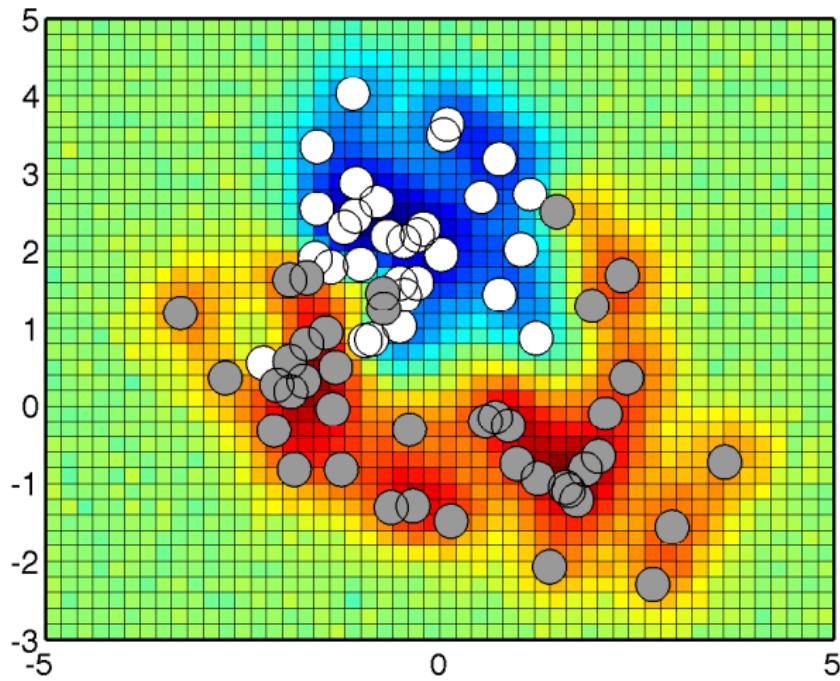


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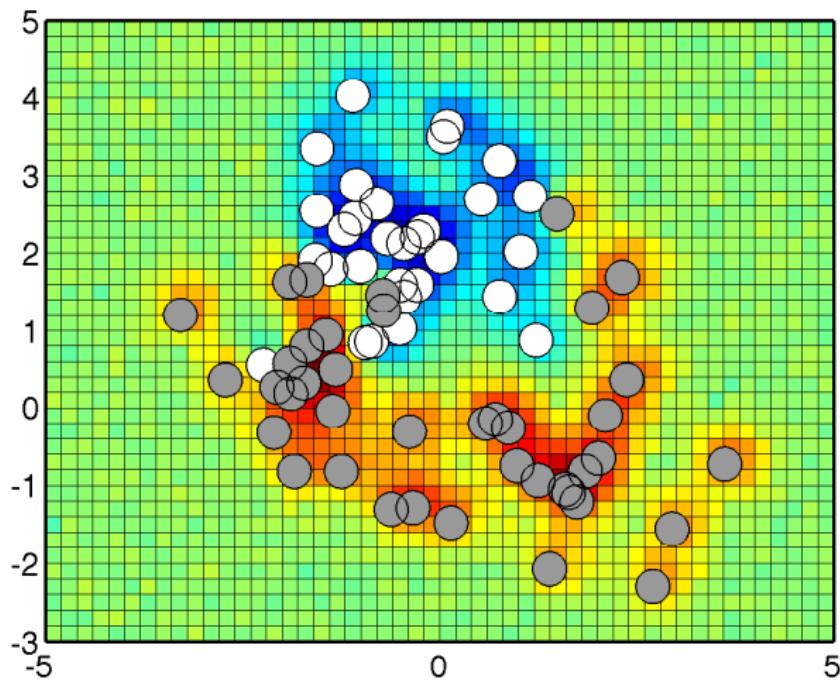


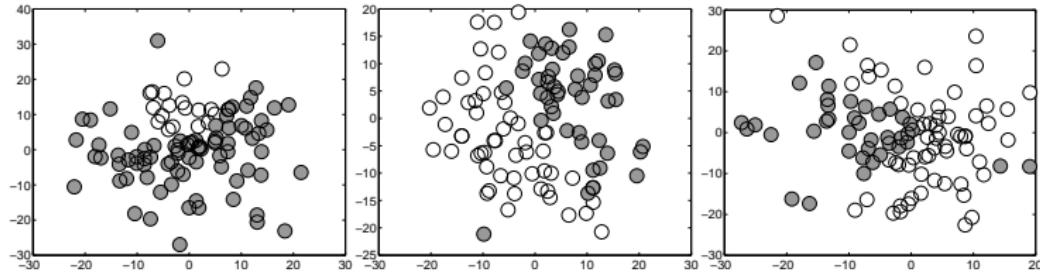
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# Note

- ▶ Inference:
  - ▶ Gibbs sampling isn't the only option
  - ▶ A popular alternative is Variational Bayes

## Note 2 – The Generative Process

- ▶ Sometimes it's useful to think of the generative process defined by the model.
- ▶ In this case, to generate  $N$  values of  $y_n$  given the associated  $x_n$ :
  - ▶ Sample  $\mathbf{f}$  from a GP with mean  $\mathbf{0}$  and Covariance matrix  $\mathbf{C}$ .
  - ▶ For each  $n = 1 \dots N$ :
    - ▶ Sample  $z_n \sim \mathcal{N}(f_n, 1)$
    - ▶ If  $z_n > 0$  set  $y_n = 1$ , otherwise  $y_n = 0$ .
- ▶ Some examples:



# GP classification exercise

## TASK [2]

- ▶ Explore GP binary classification with auxiliary variables using `gp_class_task.m`
- ▶ Try:
  - ▶ Generating data from different distributions
  - ▶ Varying covariance function and parameters
  - ▶ Taking more posterior samples
- ▶ You will also need `plotClassdata.m` and `kernel.m`

## A more general idea

- ▶ Models of this form:
  - ▶  $\mathbf{f} \sim GP$
  - ▶  $z_n \sim \mathcal{N}(f_n, 1)$
  - ▶  $P(y_n|z_n) = \delta(f(z_n))$
- ▶ Can be used for more than just binary classification.

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- ▶ Ordinal Regression:
  - ▶  $P(y_n = k|z_n)$  is now chopped at both ends:

$$P(y_n = k|z_n) = \delta(b_k < z_n < b_{k+1})$$

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  - ▶ Gibbs distribution for  $z_n$  therefore involves a Gaussian truncated at both ends.
- ▶ As well as multi-class and semi-supervised classification...

# Multi-class classification

- ▶ The previous treatment can be extended to multiple classes.
- ▶ For a problem with  $K$  classes:
  - ▶  $K$  GP priors,  $K$   $N$ -dimensional latent vectors  $\mathbf{f}_k$ .
  - ▶  $N \times K$  auxiliary variables  $z_{nk} \sim \mathcal{N}(f_{nk}, 1)$
  - ▶ And:

$$P(y_n = k | z_{n1}, \dots, z_{nK}) = \delta(z_{nk} > z_{ni} \quad \forall i \neq k)$$

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- ▶ Details of a Variational Bayes inference scheme in: **Girolami and Rogers 2006**

## Multi-class Example

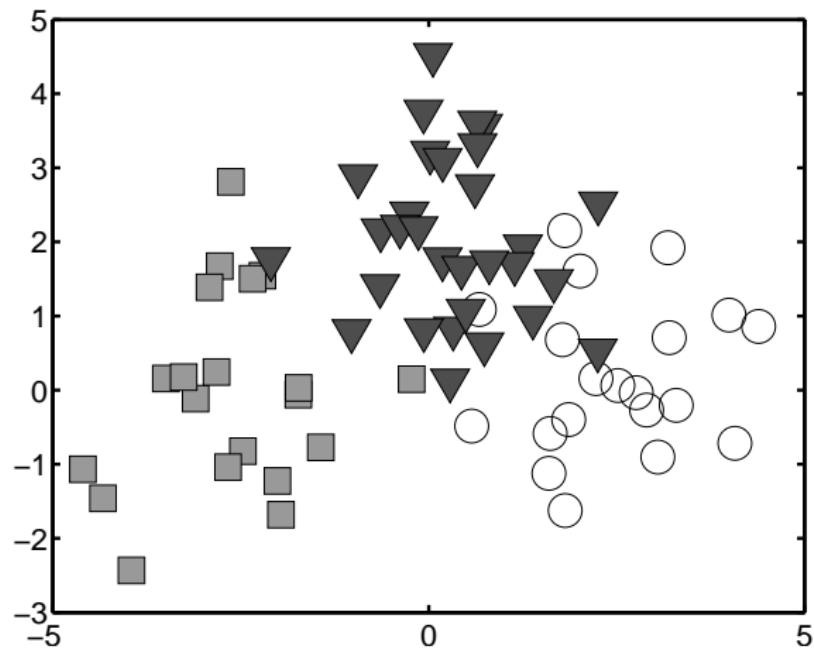


Figure 11 : Multi-class classification example. RBF covariance,  $\gamma = 1$ .

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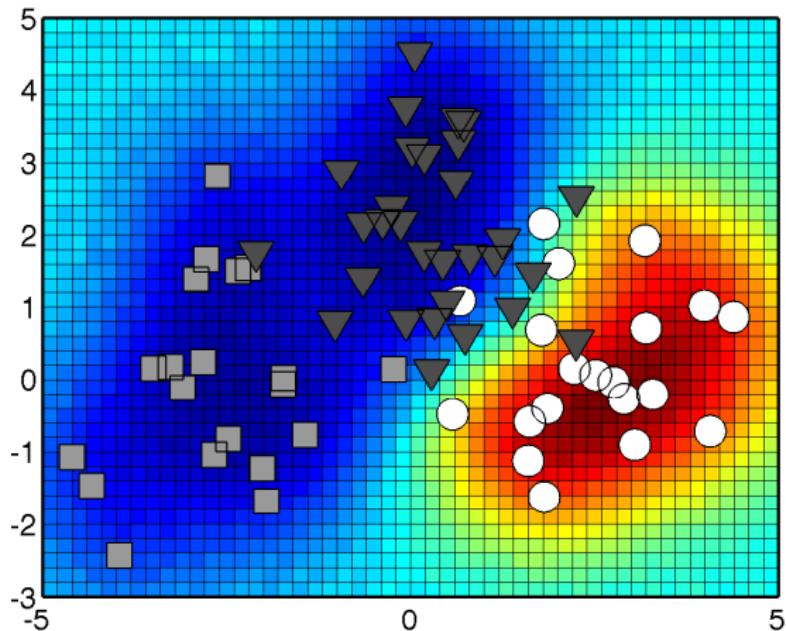


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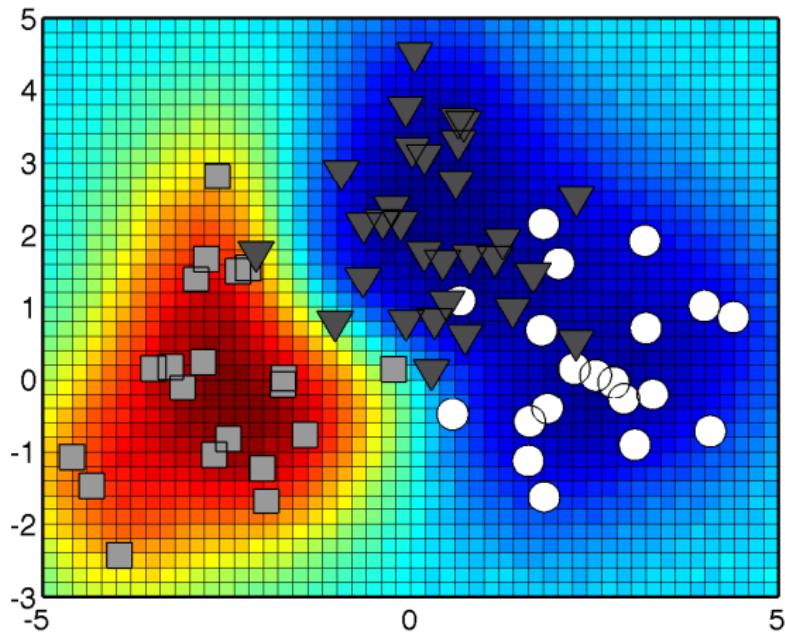


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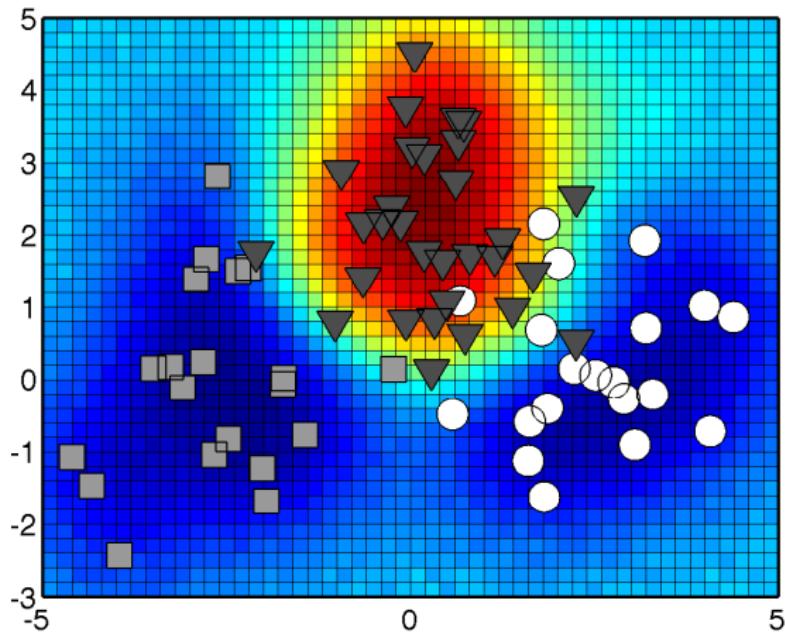


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## Semi-supervised Classification

- In some domains, only a subset of data are labeled [e.g. image classification]

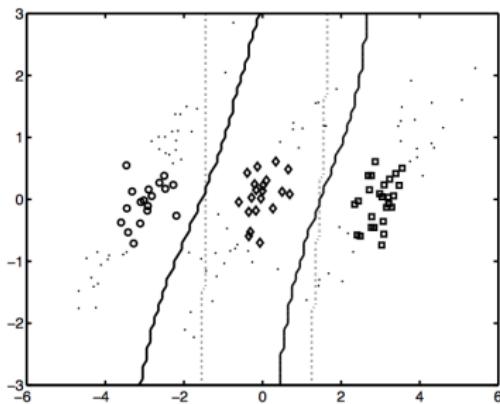
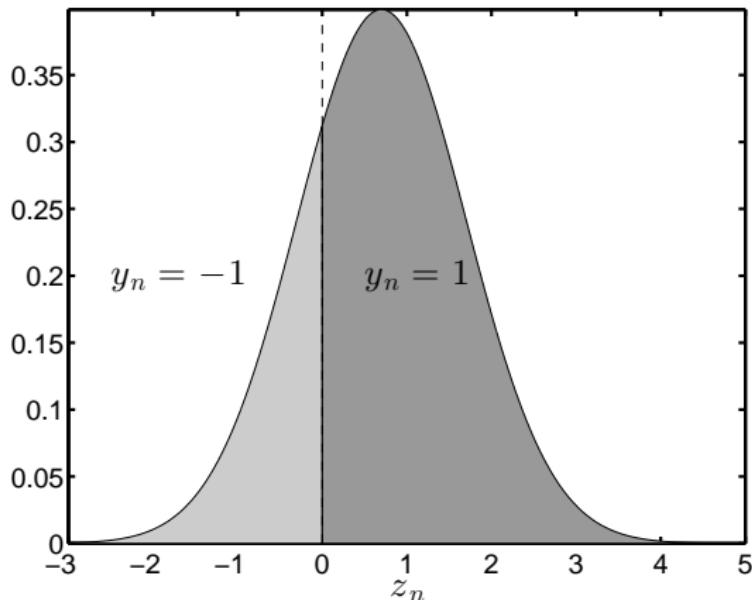


Figure 12 : A toy semi-supervised classification problem.

- Can be overcome using the Null Category Noise Model (NCNM) Lawrence and Jordan 2004

# The NCM

- ▶ Going back to binary classification, the auxiliary variable trick can be visualised:



**Figure 13 :** Visualisation of the auxiliary variable trick. The Gaussian has mean  $f_n$ . Note that I'm not calling the classes  $\pm 1$ .

# The NCNM

- To include unlabeled data, we add a third category, for  $y_n = 0$ :

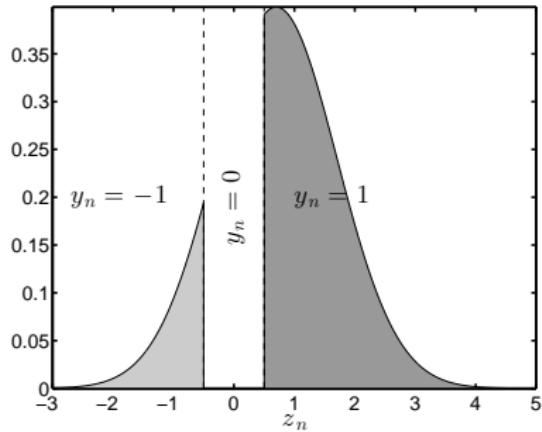


Figure 14 : Visualisation of the NCNM with a null region of width 1.

$$p(y_n|z_n) = \begin{cases} \delta(z_n < -a) & y_n = -1 \\ \delta(z_n > a) & y_n = 1 \\ \delta(z_n > -a) - \delta(z_n > a) & y_n = 0 \end{cases}$$

# The NCM

- ▶ The final step is to introduce another set of latent variables.
  - ▶  $g_n = 0$  if  $y_n$  is observed (i.e. labeled) and  $g_n = 1$  otherwise.
- ▶ And enforce the constraint that no unlabeled points can exist in the null region:

$$P(y_n = 0 | g_n = 1) = 0$$

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- ▶ This has the effect of introducing an empty region around the decision boundary
  - ▶ i.e. pushing the decision boundary into regions of empty space
- ▶ Inference:
  - ▶ Gibbs sampling is the same as the binary case except  $z_n | f_n, g_n = 1$ .
  - ▶ This is a mixture of two truncated Gaussians – sample the component, and then sample  $z_n$ .

## NCNM Example

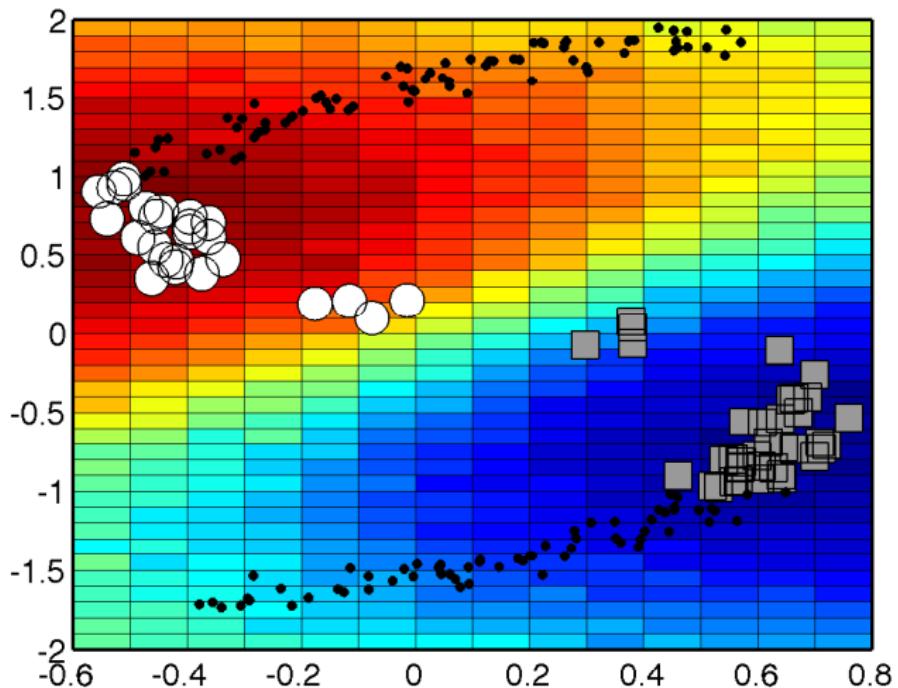


Figure 15 : Standard GP classification (unlabeled data ignored)

## NCNM Example

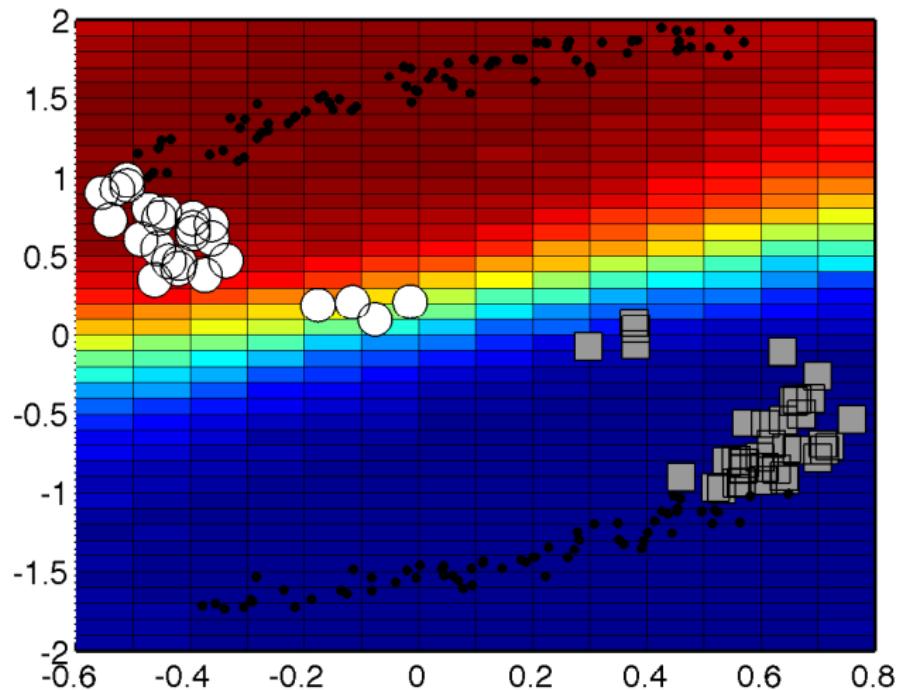


Figure 16 : NCNM GP classification

# NCNM Exercise

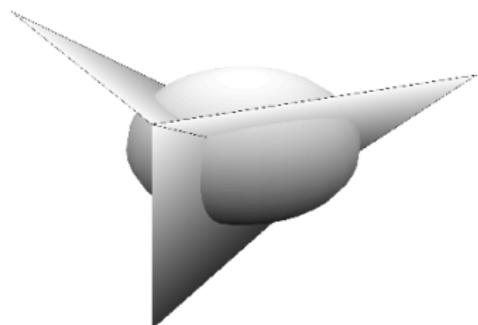
## TASK [3]

- ▶ Experiment with the NCNM using `gp_ncnm_task.m`
- ▶ Setting  $a=0$  results in the standard model
- ▶ Setting  $a>0$  uses the NCNM
- ▶ It's not always easy to get the results you want to see!

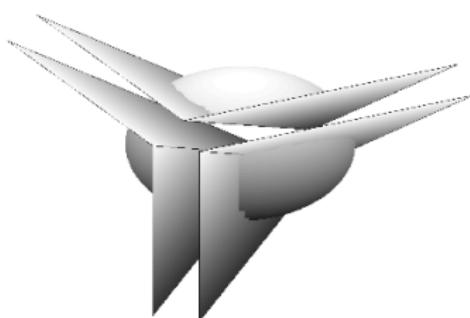
## Multi-class NCM

- ▶ This idea can be extended to the multi-class setting.
- ▶ See [Rogers and Girolami 2007](#)

$$P(y_n = k | z_{n1}, \dots, z_{nK}) = \begin{cases} \delta(z_{nk} > z_{ni} + a \quad \forall i \neq k) & y_n > 0 \\ 1 - \sum_j \delta(z_{nj} > z_{ni} + a \quad \forall i \neq j) & y_n = 0 \end{cases}$$



(a) A visualisation of the truncation caused by the standard multi-class probit model



(b) A visualisation of the truncation caused by the multi-class probit model with a null region

Figure 17 : Visualisation of truncation

# Summary

- ▶ GP priors aren't restricted to regression.
- ▶ Analytical solutions aren't possible
- ▶ Auxiliary Variable Trick makes inference (via Gibbs sampling or Variational Bayes) straightforward for:
  - ▶ Binary classification
  - ▶ Ordinal regression
  - ▶ Multi-class classification
  - ▶ Semi-supervised classification (binary and multi-class)
  - ▶ As well as others (e.g. binary PCA)

# Lecture 5: Application: Clinical Ratings

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## Clinicians disagree in AandE

- ▶ Patients in Accident and Emergency (A&E) are continually monitored.
  - ▶ Heart rate
  - ▶ Blood pressure
  - ▶ Temperature
  - ▶ etc

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  - ▶ A (healthy(ish)), B, C, D, E, F (critical)

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- ▶ Patients in A&E are continually monitored.
  - ▶ Heart rate
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  - ▶ etc
- ▶ Based on these hourly observations, clinicians (in a Glasgow hospital) give each patient an ordinal rating
  - ▶ A (healthy(ish)), B, C, D, E, F (critical)
- ▶ These ratings are *subjective*
  - ▶ How do clinicians disagree? (variance? bias?)
- ▶ More details of this work in [Rogers et al 2013](#) and [Rogers et al 2010](#)

## Data

- ▶  $c = 1 \dots C$  clinicians.
- ▶  $p = 1 \dots P$  patients.
- ▶ For patient  $p$ , we have  $T_p$  observations at times  $\mathbf{t}_p = [t_{p1}, \dots, t_{pT_p}]^T$ .
- ▶  $y_{\tau c}^p$  is rating at  $t_{p\tau}$  ( $\{A, B, C, D, E\}$ ).

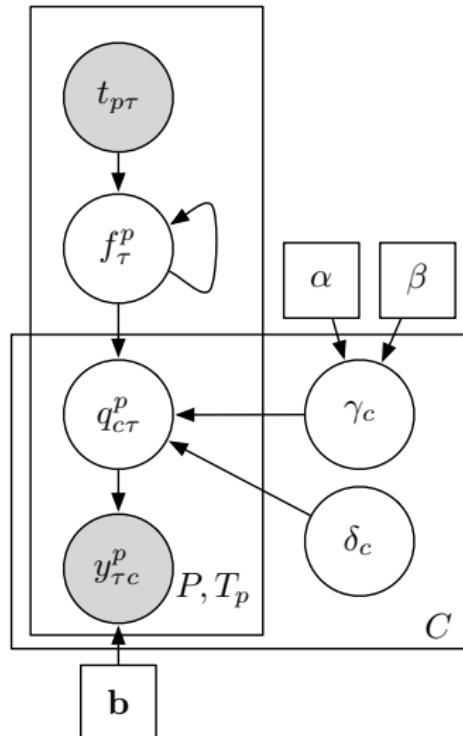
# The model

- ▶ Assumptions:
  - ▶ We assume that there is an unobserved continuous latent health function for each patient
  - ▶ Each clinician observes this and corrupts it in two ways:
    - ▶ Adds Gaussian noise
    - ▶ Adds a constant offset (optimist, pessimist)
  - ▶ Corrupted health is then binned to give category

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  - ▶ Corrupted health is then binned to give category
- ▶ The model:
  - ▶ Patient health is modelled as a GP.
  - ▶ Corrupted health is the auxiliary variable ( $q$ )
  - ▶  $q$  is binned to produce rating.
  - ▶ Note that  $p(q|f)$  has been generalised from standard normal.

# Model



$$\mathbf{f}^p \sim \mathcal{N}(\mathbf{0}, \mathbf{C}^p) \text{ [health]}$$

$$\delta_c \sim \mathcal{N}(0, 1) \text{ [offset]}$$

$$\gamma_c \sim \mathcal{G}(\alpha, \beta) \text{ [precision]}$$

$$q_{c\tau}^p \sim \mathcal{N}(f_\tau^p + \delta_c, \gamma_c^{-1})$$

$$P(y_{\tau c}^p = k) = \delta(b_k < q_{c\tau}^p < b_{k+1})$$

Previously auxiliary variables were  $z_n \sim \mathcal{N}(f_n, 1)$ . This model adds clinician-specific offsets and precisions:

$$q_{c\tau}^p \sim \mathcal{N}(f_\tau^p + \delta_c, \gamma_c^{-1}).$$

Figure 18 : Plates diagram

## Example data generation

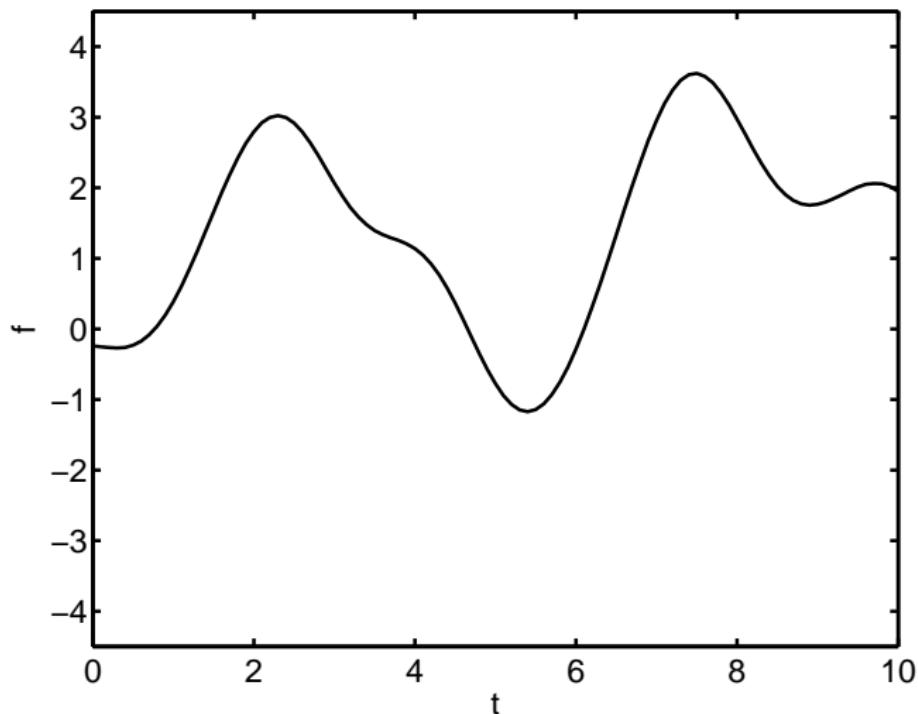


Figure 19 : Example of the generative process described by the model for three clinicians.

## Example data generation

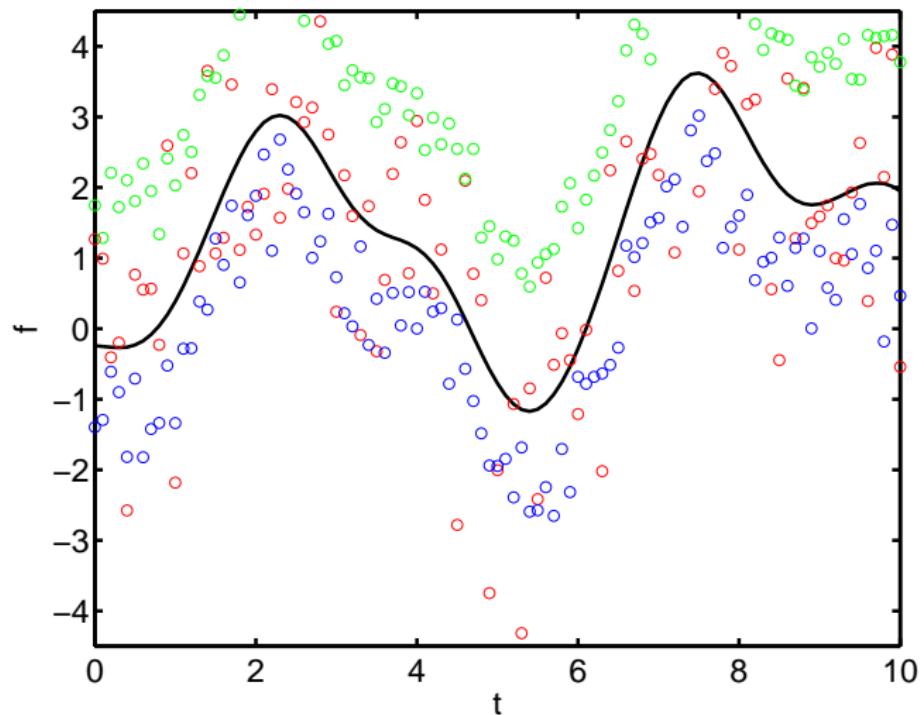


Figure 19 : Example of the generative process described by the model for three clinicians.

## Example data generation

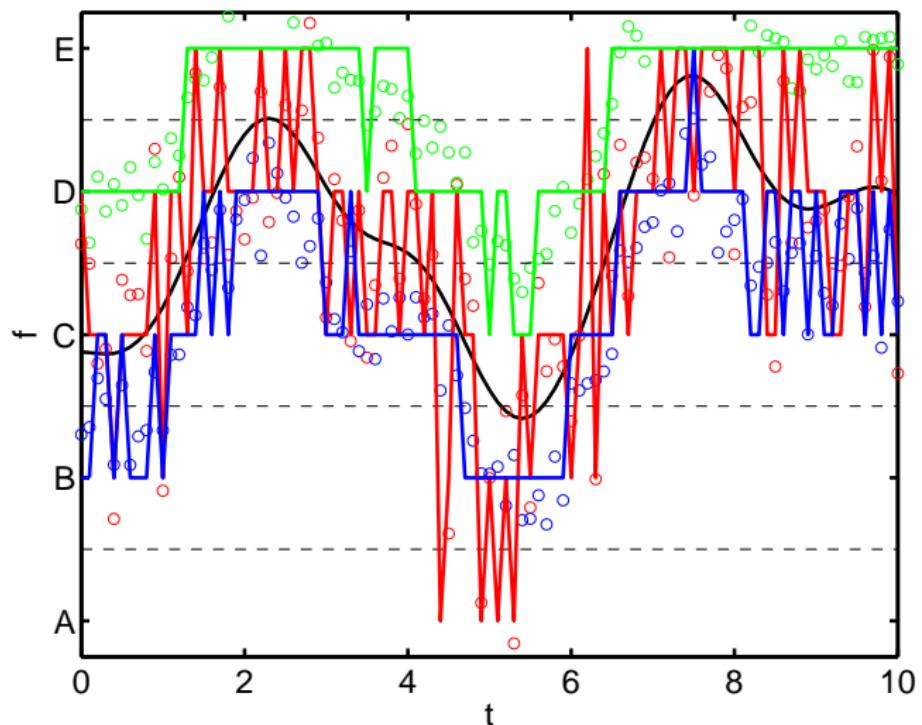


Figure 19 : Example of the generative process described by the model for three clinicans.

## Model inference

- ▶ Gibbs sampling is straightforward
- ▶ We sample:
  - ▶ The latent health function for each patient.
  - ▶ The auxiliary variables.
  - ▶ The offset and precision for each clinician.

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  - ▶ The offset and precision for each clinician.
- ▶ The offset and precision tell us how the clinicians disagree.
- ▶ Identifiability: offset for one clinician fixed to 0.

## Results

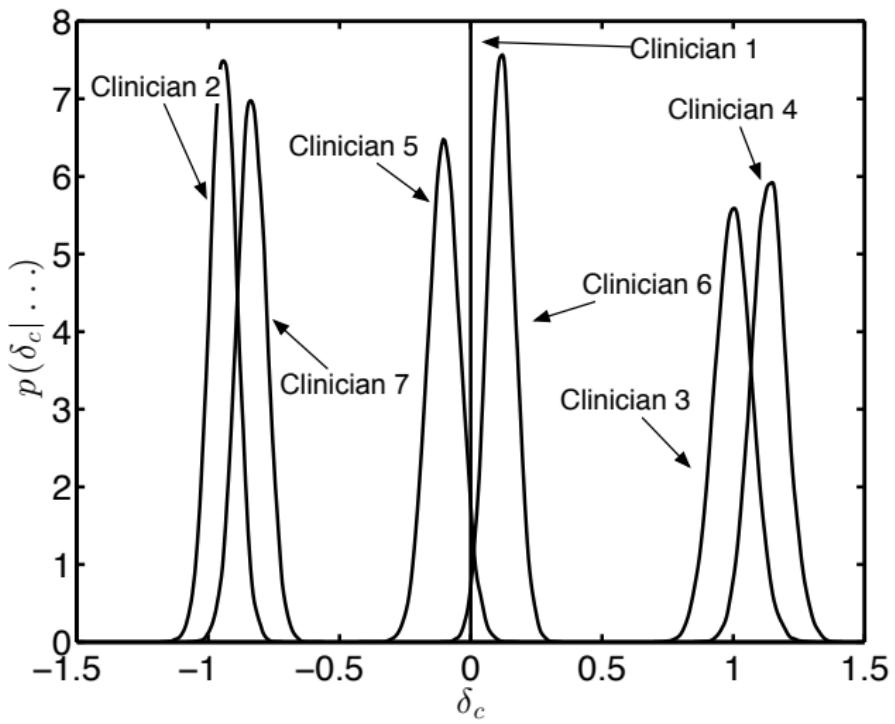


Figure 20 : Marginal offset posteriors

## Results

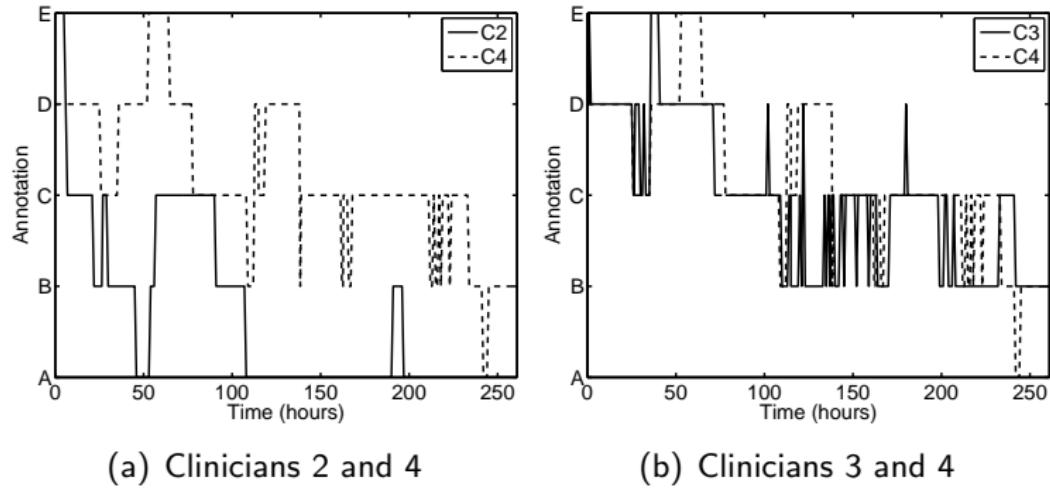


Figure 21 : Inferred offsets make sense on inspection of the data.

## Results

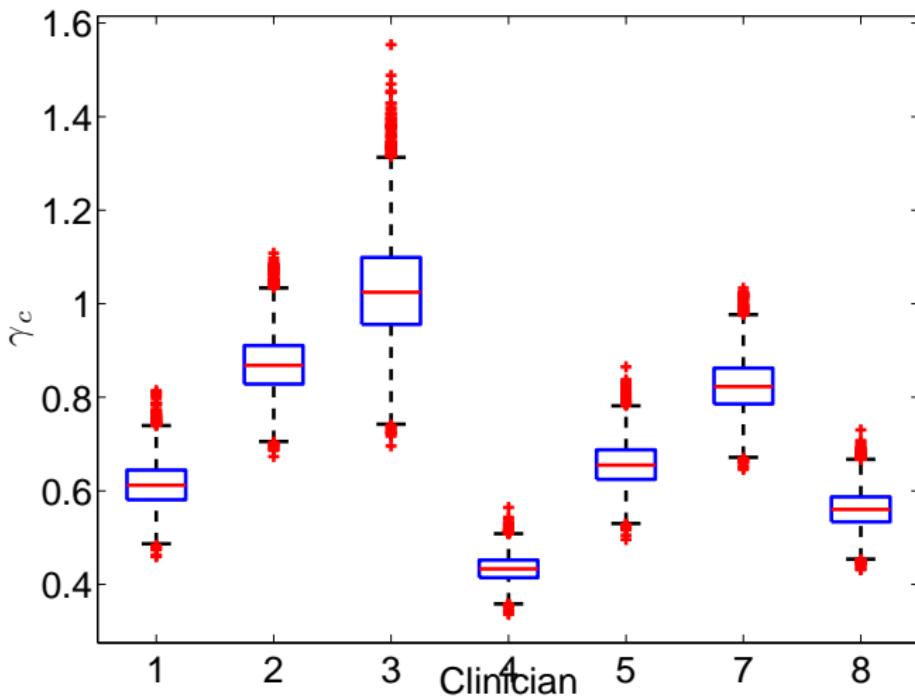
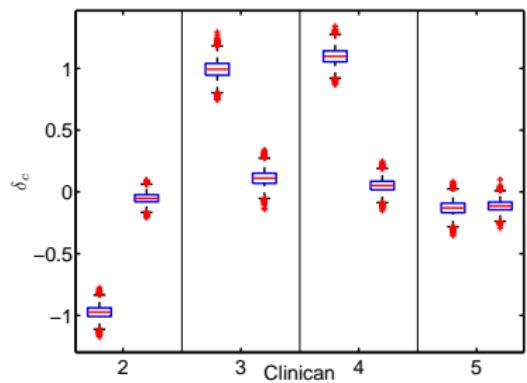


Figure 22 : Marginal precision posteriors. Clinicians 1, 4, and 8 appear to be the least consistent (wrt the majority)

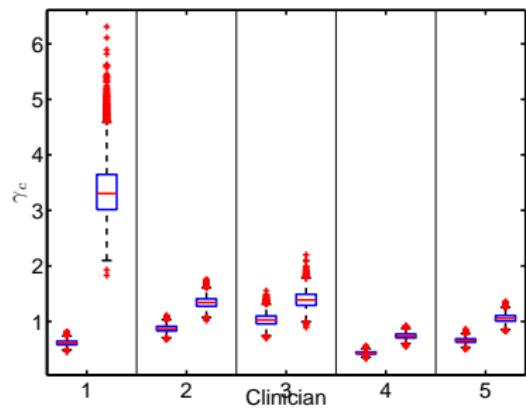
# INSIGHT

- ▶ After the initial annotation, clinicians went through INSIGHT procedure.
- ▶ The goal was to make ratings more consistent.
- ▶ If it succeeded, we should see a reduction in offset and increase in precision in the post-INSIGHT data.

# Post-INSIGHT results



(a) Offsets

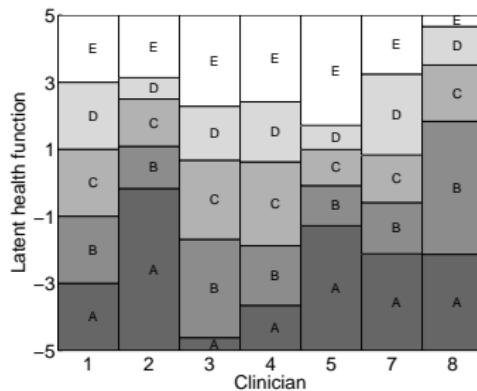


(b) Precisions

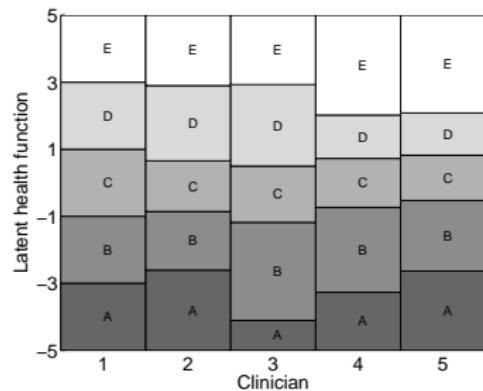
Figure 23 : Offsets and precision before and after INSIGHT. Offsets get closer to 0, whilst precision increase suggesting greater agreement amongst clinicians.

# Inferring category boundaries

- ▶ So far, it has been assumed that all categories are the same size (i.e. the elements of  $\mathbf{b}$  are equally spaced).
- ▶ We can also infer these (with fixed end-points and  $\delta_c = 0$ ).
- ▶ Removes uniform prior assumption over categories.



(a) Before INSIGHT



(b) After INSIGHT

Figure 24 : Posterior mean category boundaries.

## Summary and Conclusions

- ▶ Model allows us to:
  - ▶ learn something about *how* clinicians disagree and how they rate.
  - ▶ assess the effectiveness of the INSIGHT procedure.

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- ▶ GP prior:
  - ▶ Flexible
  - ▶ Required no parametric assumptions about health function
  - ▶ Hyper-parameter ( $\gamma$ ) was inferred in the model (could be patient-specific)
- ▶ Auxiliary Variable Trick:
  - ▶ Not restricted to a standard Gaussian centered on the GP variable.
  - ▶ Incorporated offset and precision without causing additional inference challenges.