Non-parametric Bayesian Methods in Machine Learning

Dr. Simon Rogers
School of Computing Science
University of Glasgow
simon.rogers@glasgow.ac.uk
@sdrogers

April 29, 2014

Outline

- **FIX ME AT THE END**
- (My) Bayesian philosophy
- Gaussian Processes for Regression and Classification
  - GP preliminaries
  - Classification (including semi-supervised)
  - Regression application 1: clinical (dis)-agreement
  - Regressopn application 2: typing on touch-screens
- Dirichlet Process flavoured Cluster Models
  - DP preliminaries
  - Idenfitying metabolites
  - (if time) Cluster models for multiple data views

About me

- I'm not a statistican 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 1: Bayesian Inference

Dr. Simon Rogers
School of Computing Science
University of Glasgow
simon.rogers@glasgow.ac.uk
@sdrogers

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Bayesian Inference

Standard setup:

- We have some data $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
- We have a model $p(\mathbf{X}|\mathbf{\Theta})$
- We define a prior $p(\mathbf{\Theta})$

Bayesian Inference

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- We have a model $p(\mathbf{X}|\mathbf{\Theta})$
- We define a prior $p(\mathbf{\Theta})$
- We use Bayes rule (and typically lots of computation) to compute (or estimate) the posterior:

$$p(\mathbf{\Theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\mathbf{\Theta})p(\mathbf{\Theta})}{p(\mathbf{X})}$$

Why be Bayesian?

Why be Bayesian?

- Within ML we are often interested in making predictions (predicing y_* from $\mathbf{x}_*$).
- Being Bayesian allows us to *average* over uncertainity in parameters when making predictions:

$$p(y_*|\mathbf{x}_*, \mathbf{X}) = \int p(y_*|\mathbf{x}_*, \boldsymbol{\Theta}) p(\boldsymbol{\Theta}|\mathbf{X}) \; d\boldsymbol{\Theta}$$

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- Bayes rule tells us how this uncertainty should change as data appear.

Lecture 2: Gaussian Process Basics

Dr. Simon Rogers
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University of Glasgow
simon.rogers@glasgow.ac.uk
@sdrogers

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Gaussian Processes

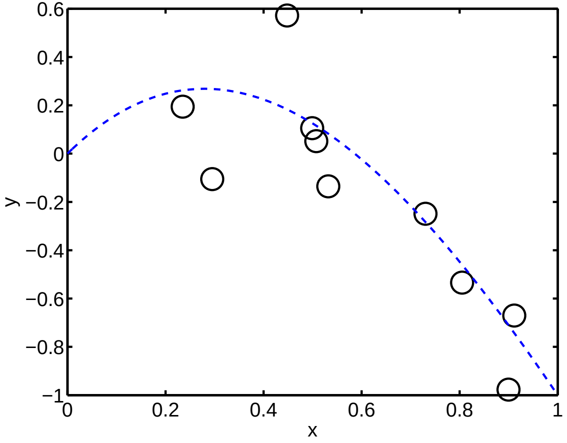

Figure 1 : A familiar problem: learn the underlying function (blue) from the observed data (crosses).

A parametric approach?

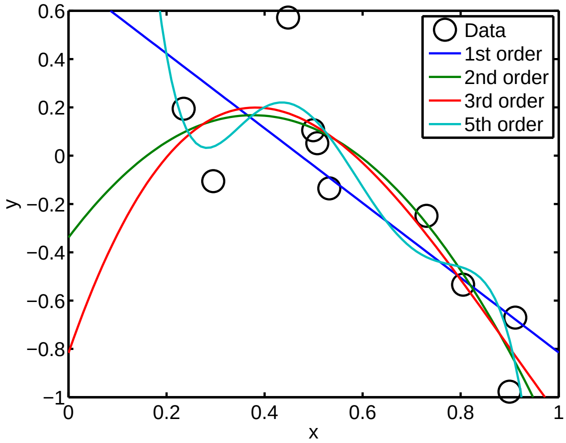

Figure 2 : Polynomials fitted by least squares.

It's easy to under and over-fit. What if we have no idea of the parametric form of the function?

A non-parametric approach - Gaussian Processes

- Rather than forcing us to choose a particular parametric form, a Gaussian Process (GP) allows us to place a prior distribution directly on *functions*
- With a GP prior we can:
  - Sample functions from the prior
  - Incorporate data to get a *posterior* distribution over functions
  - Make predictions

Visual example – prior

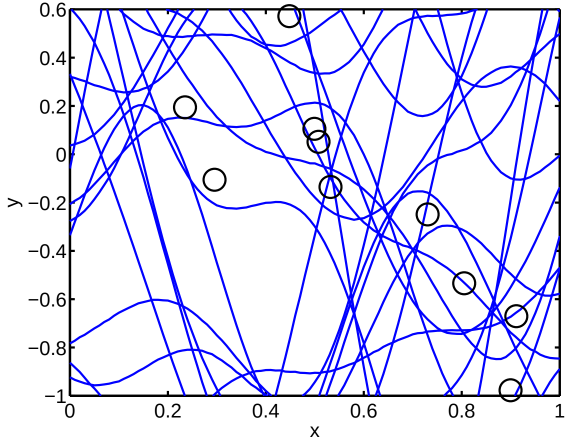

Figure 3 : Some functions drawn from a GP prior.

Visual exmample – posterior

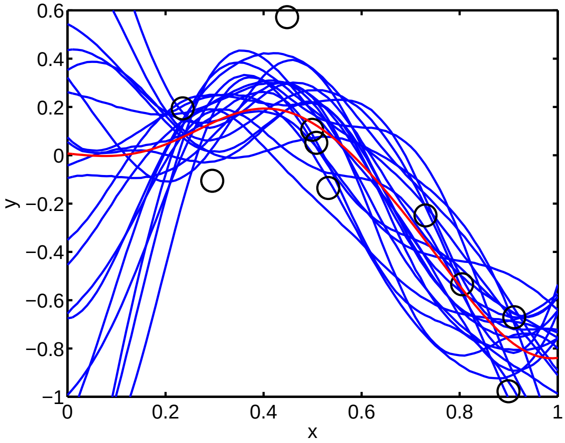

Figure 4 : Some functions drawn from the GP posterior. Posterior mean is shown in red.

Visual example – predictions

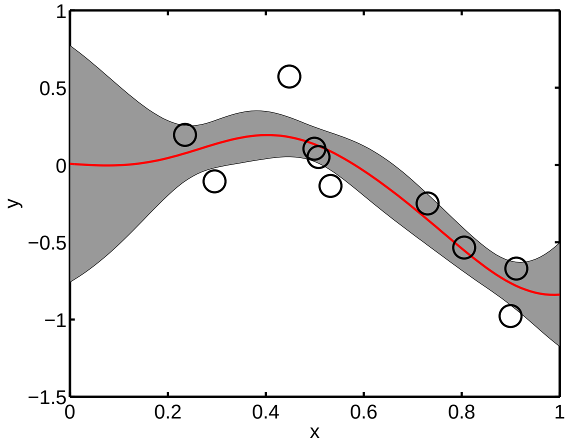

Figure 5 : Predictive mean and standard deviations.

Some formalities

- We observe N training points, each of which consists of a set of features $\mathbf{x}_n$ and a target y_n.
- We can stack all of the y_n into a vector and $\mathbf{x}_n$ into a matrix:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix}$$

GP definition

- The GP assumes that the vector of *all possible* y_n is a draw from a Multi-Variate Gaussian (MVG).
- We don't observe *all possible* values (if we did, we wouldn't need to make predictions!)

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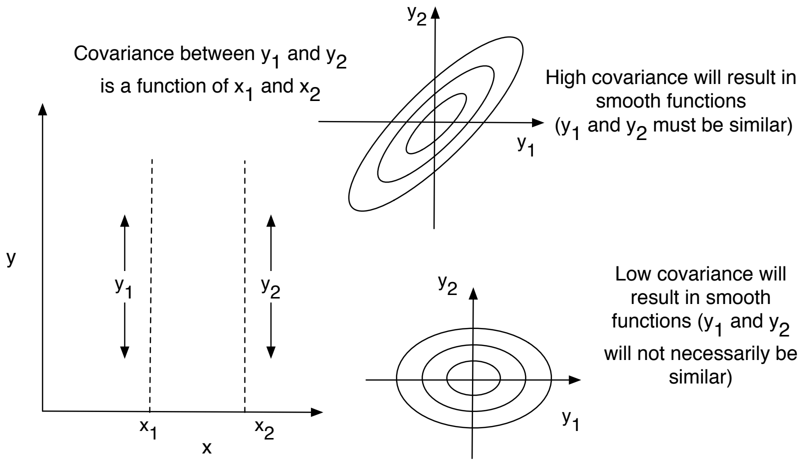
- i.e. if we have N training points, we're dealing with an N-dimensional MVG
- With mean $\boldsymbol{\mu}$ (normally 0) and covariance $\mathbf{C}$
- $\mathbf{x}_n$ looks to have disappeared – we find it inside $\mathbf{C}$

GP definition



Covariance between y_1 and y_2 is a function of x_1 and x_2
y
y_1
y_2
x_1
x_2
x
y_2
y_1
High covariance will result in smooth functions (y_1 and y_2 must be similar)
y_2
y_1
Low covariance will result in smooth functions (y_1 and y_2 will not necessarily be similar)

Figure 6 : Schematic of GP prior for two function values.

Covariance functions

- By choosing a covariance function, we are making an assumption on the *smoothness* of the regression function.
- Common choices:
  - Linear: $C(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1^T \mathbf{x}_2$
  - RBF: $C(\mathbf{x}_1, \mathbf{x}_2) = \exp\left\{-0.5\gamma ||\mathbf{x}_1 - \mathbf{x}_2||^2\right\}$
  - And many, many more.
- More details: `http://www.gaussianprocess.org/gpml/`
  - (Free) book
  - Code

Hyper-parameters

$$C(\mathbf{x}_1, \mathbf{x}_2) = \exp\left\{-0.5\gamma||\mathbf{x}_1 - \mathbf{x}_2||^2\right\}$$

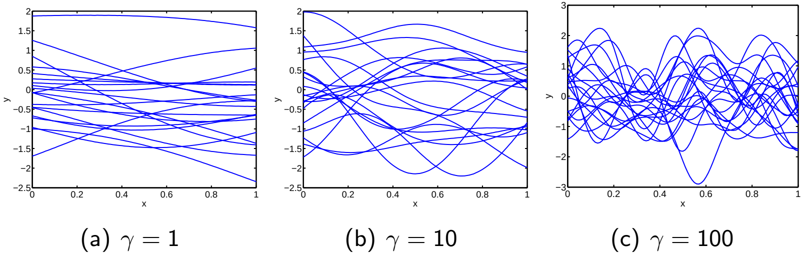


Figure 7 : Varying hyper-parameters in an RBF covariance varies the smoothness of the function.

Optimising hyper-parameters

Making predictions

- If we assume no observation noise, we can place GP prior directly on $\mathbf{y}$
- If we observe $\mathbf{y}$ and want to predict y_* for a new observation $\mathbf{x}_*$:
  - Construct joint Density (it's a Gaussian):

$$\left[\begin{array}{c} \mathbf{y} \\ y_* \end{array}\right] \sim \mathcal{N}\left(\mathbf{0}, \left[\begin{array}{cc} C(\mathbf{X},\mathbf{X}) & C(\mathbf{X},\mathbf{x}_*) \\ C(\mathbf{x}_*,\mathbf{X}) & C(\mathbf{x}_*,\mathbf{x}_*) \end{array}\right]\right)$$

  - And then use standard results for Gaussian conditionals:

$$p(y_*|\mathbf{y},\mathbf{X},\mathbf{x}_*) = \mathcal{N}(\mu_*,\sigma_*^2)$$

where

$$\begin{aligned} \mu_* &= C(\mathbf{x}_*,\mathbf{X})C(\mathbf{X},\mathbf{X})^{-1}\mathbf{y} \\ \sigma_*^2 &= C(\mathbf{x}_*,\mathbf{x}_*) - C(\mathbf{x}_*,\mathbf{X})C(\mathbf{X},\mathbf{X})^{-1}K(\mathbf{X},\mathbf{x}^*) \end{aligned}$$

`http://orion.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf`

Noise-free example

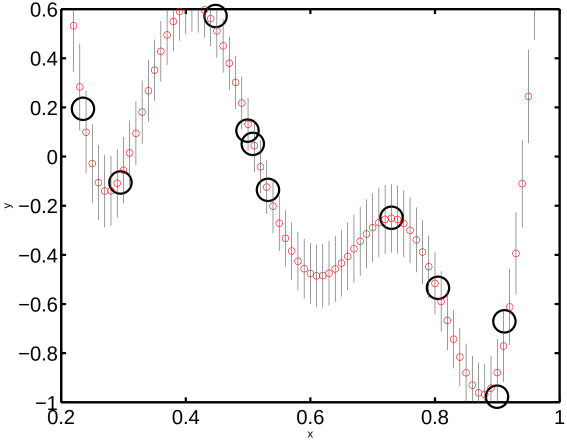


Figure 8 : $\mu_* \pm \sigma_*$ for a noise-free GP at lots of test points

Predictions with noise

- Assuming Gaussian observation noise, we introduce a set of latent variables, f_n and place the GP prior on these.

$$y_n \sim \mathcal{N}(f_n, \sigma^2), \quad \mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$

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$$y_n \sim \mathcal{N}(f_n, \sigma^2), \quad \mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$

- Because both terms are Gaussian, the noise can be pushed into the covariance function:

$$\begin{bmatrix} \mathbf{y} \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} C(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbf{I} & C(\mathbf{X}, \mathbf{x}_*) \\ C(\mathbf{x}_*, \mathbf{X}) & C(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix}\right)$$

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- And, as before (except now predicting f_*):

$$p(f_* | \mathbf{y}, \mathbf{X}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(\mu_*, \sigma_*^2)$$

where

$$\begin{aligned} \mu_* &= C(\mathbf{x}_*, \mathbf{X}) \left[C(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbf{I} \right]^{-1} \mathbf{y} \\ \sigma_*^2 &= C(\mathbf{x}_*, \mathbf{x}_*) - C(\mathbf{x}_*, \mathbf{X}) \left[C(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbf{I} \right]^{-1} K(\mathbf{X}, \mathbf{x}^*) \end{aligned}$$

Example with noise

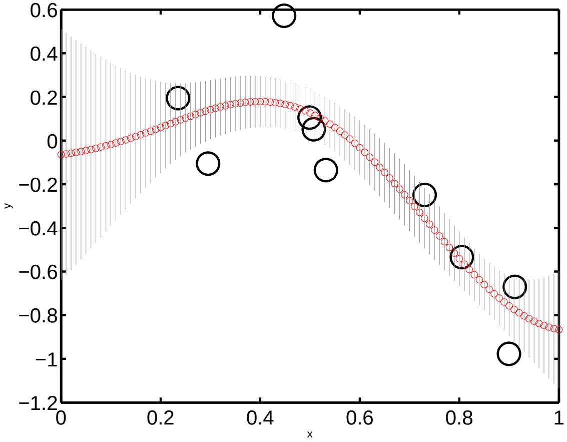

Figure 9 : $\mu_* \pm \sigma_*$ at lots of test points when observation noise is included.

Lecture 3: Application: Touchscreen typing

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@sdrogers

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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:
  - Add some

Background 2: All users are different

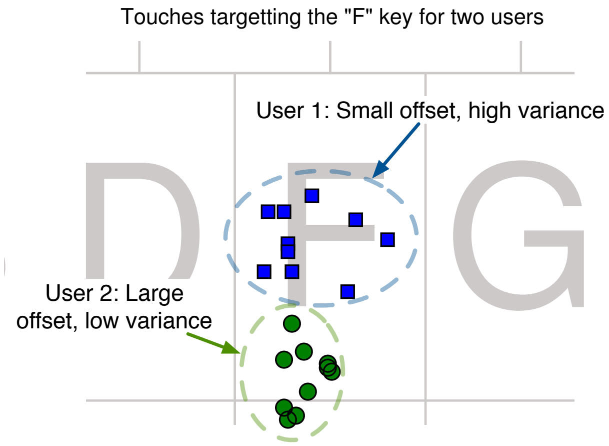


Figure 10 : Touches recorded by two users aiming for the ‘F’ key. User 2 has high bias and low variance, user 1 has low bias and high variance.

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 $\rightarrow$ 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.

Our idea

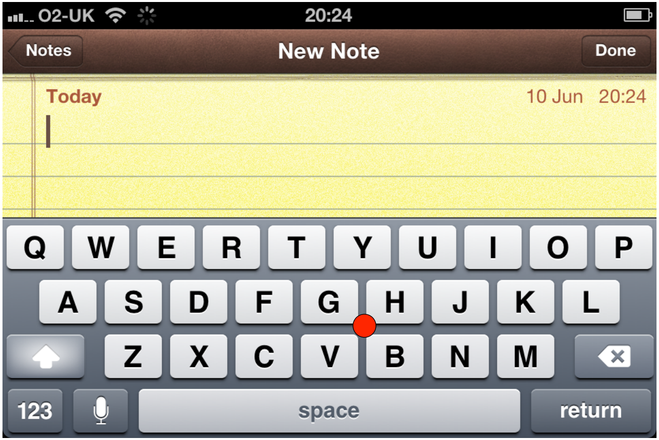
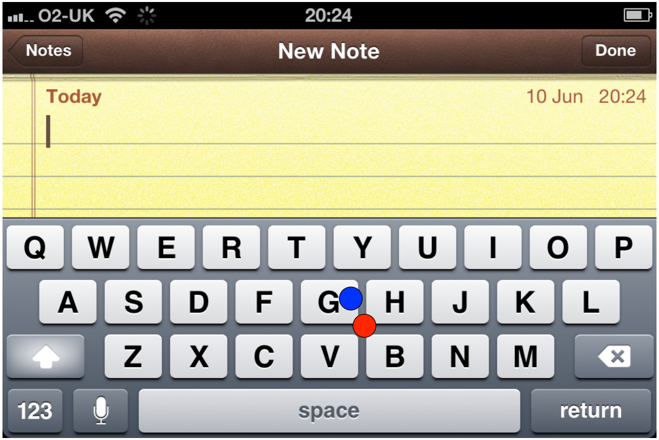


Figure 11 : Train GPs to predict the intended touch from an input touch. The flexibility of GPs means that the mean and covariance of the offset can vary across the keyboard.

Our idea



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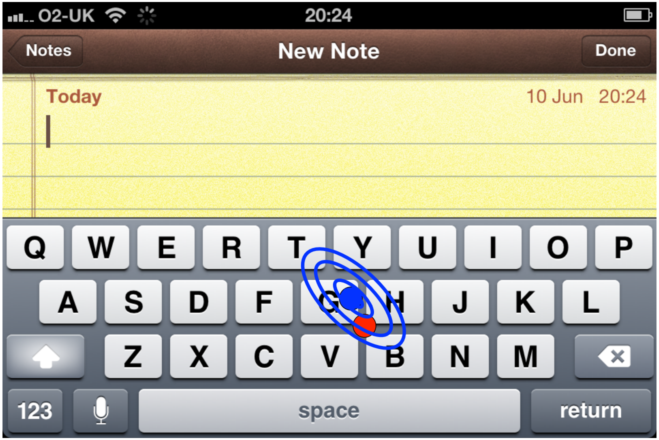

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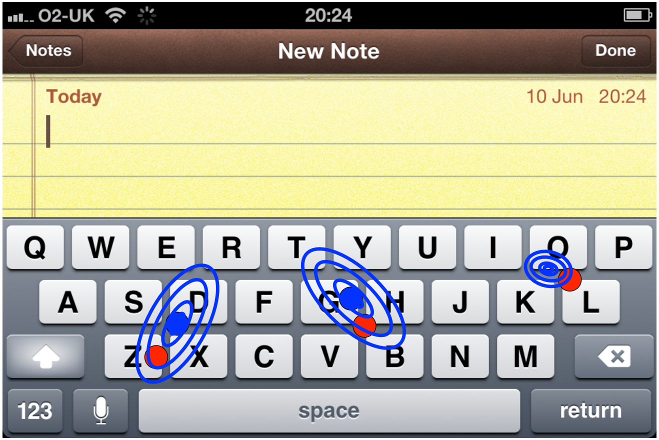

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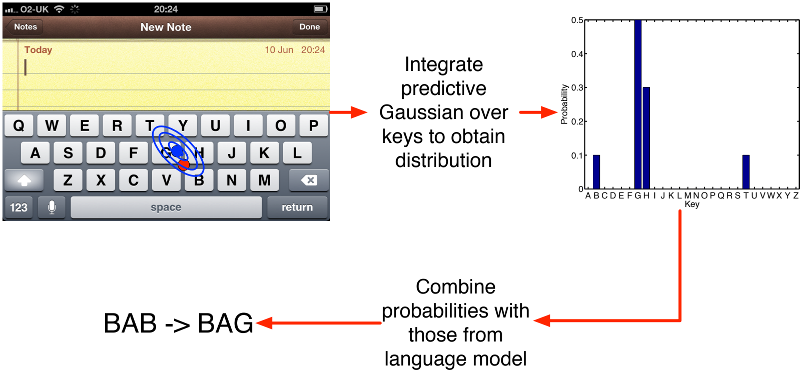

O2-UK
20:24
Notes
New Note
Done
Today
10 Jun 20:24
Q W E R T Y U I O P
A S D F G H J K L
Z X C V B N M
123
space
return
Integrate predictive Gaussian over keys to obtain distribution
Probability
0.5
0.4
0.3
0.2
0.1
0
A B C D E F G H I J K L M N O P Q R S T U V W X Y Z
Key
Combine probabilities with those from language model
BAB -> BAG

Figure 12 : The complete system

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. Target: the center of the intended key minus the touch (i.e. the offset).

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  - Data: the x, y location of the recorded touch. Target: the center of the intended key minus the touch (i.e. the offset).
- Used a GP with zero mean and a composite covariance:

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

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- 10 participants, each did $3\times$ 45 minute sessions, typing whilst sitting, standing and walking. [more details in paper]

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- 10 participants, 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

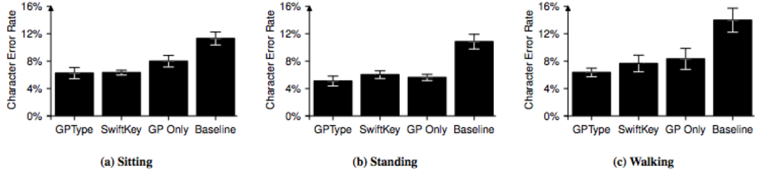

Figure 4. Character error rates for the two keyboards we evaluated, separated by mobility condition (Study 2). Plots show mean and standard error across all participants. The baseline method represents the literal keys touched, while GP Only shows the keys hit after the mean GP offset is applied.

Figure 13 : Results of GPType experiment

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

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)certainity is passed to the SLM
- Performance is promising

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- Performance is promising
- Also in the paper:
  - Using *pressure* to allow users *explicit* control of variance. Allows users to switch SLM off (when tying slang / names etc) or rely on it more for words they think it will get right (humans are quite good at predicting auto-correct errors).

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- More info:
  - `http://www.youtube.com/watch?v=1lQI5gV5l74`
  - `http://pokristensson.com/pubs/WeirEtAlCHI2014.pdf`
  - Acknowledgements: Daryl Weir, Per Ola Kristensson, Keith Vertanen, Henning Pohl

Lecture 4: GPs for classification and ordinal regression

Dr. Simon Rogers
School of Computing Science
University of Glasgow
simon.rogers@glasgow.ac.uk
@sdrogers

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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 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 $z_n | f_n, y_n$:

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

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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

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

- 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

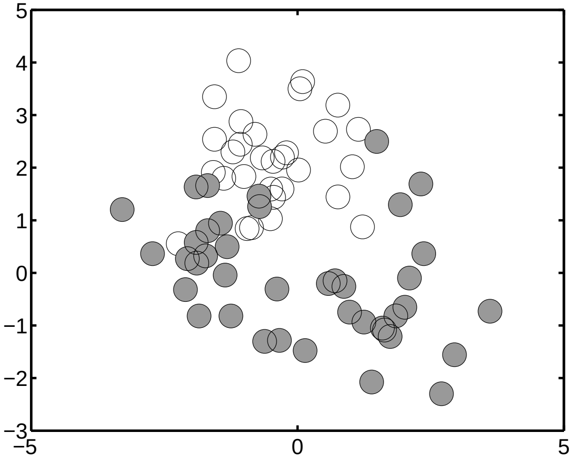

Figure 14 : Some simple classification data

Example - binary classification

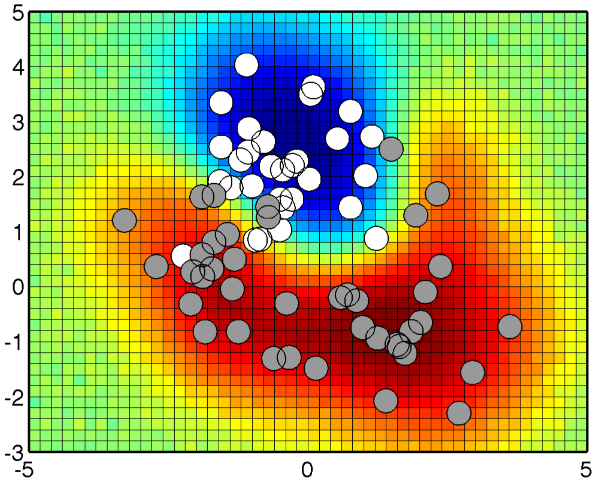

Figure 15 : Predictive probabilities averaged over 1000 Gibbs samples using an RBF covariance. As γ is increased, the model overfits.

Example - binary classification

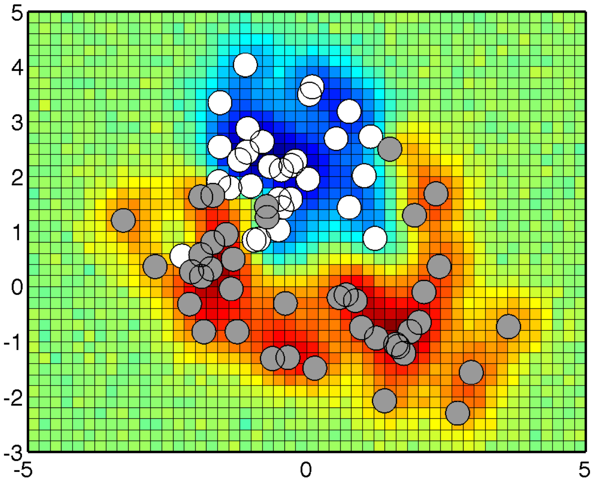

Figure 15 : Predictive probabilities averaged over 1000 Gibbs samples using an RBF covariance. As γ is increased, the model overfits.

Example - binary classification

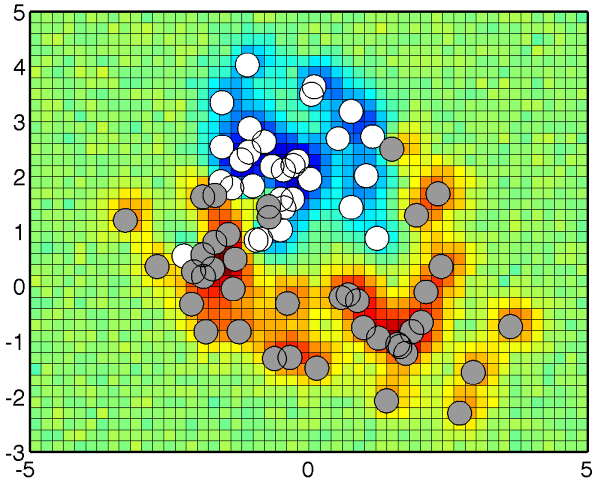

Figure 15 : Predictive probabilities averaged over 1000 Gibbs samples using an RBF covariance. As γ is increased, the model overfits.

Other things

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

Other things

- Inference:
  - Gibbs sampling isn't the only option
  - A popular alternative is Variational Bayes
- Ordinal Regression:
  - Inference for ordinal regression follows the same process.
  - The only difference lies in $P(y_n|z_n)$:

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

  - Gibbs distribution for z_n therefore involves a Gaussian truncated at both ends.

Lecture 5: Application: Clinical Ratings

Dr. Simon Rogers
School of Computing Science
University of Glasgow
simon.rogers@glasgow.ac.uk
@sdrogers

April 29, 2014

Clinicians disagree in AandE

- blah