Non-parametric Bayesian Methods in Machine Learning

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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

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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 $p(\mathbf{\Theta})$

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- We have a model $p(X|\Theta)$
- We define a prior $p(\Theta)$
- ► 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?

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- ▶ 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:

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

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

Lecture 2: Gaussian Process Basics

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Gaussian Processes

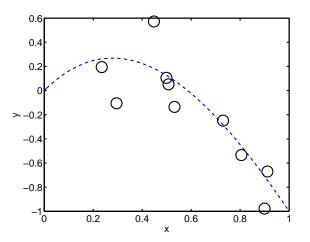


Figure 1: A familiar problem: learn the underlying function (blue) from the observed data (crosses).

A parametric approach?

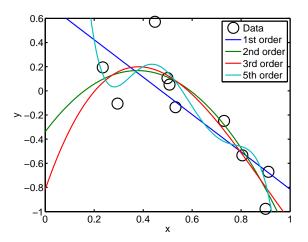


Figure 2: Polynomials fitted by least squares.

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

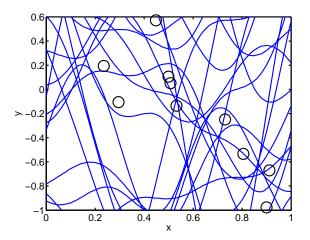


Figure 3: Some functions drawn from a GP prior.

Visual exmample – posterior

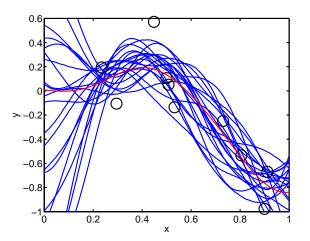


Figure 4: Some functions drawn from the GP posterior. Posterior mean is shown in red.

Visual example – predictions

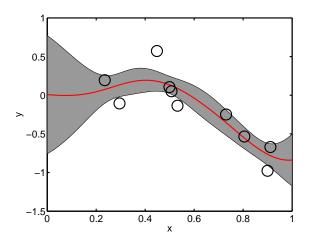


Figure 5: Predictive mean and standard deviations.

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:

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

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- \triangleright \mathbf{x}_n looks to have disappeared we find it inside **C**

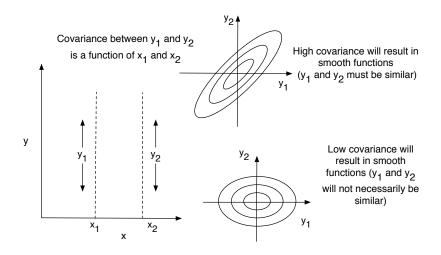


Figure 6: Schematic of GP prior for two function values.

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: $C(\mathbf{x}_1, \mathbf{x}_2) = \exp\{-0.5\gamma ||\mathbf{x}_1 \mathbf{x}_2||^2\}$
 - And many, many more.
- ► More details: http://www.gaussianprocess.org/gpml/
 - ► (Free) book
 - Code

Hyper-parameters

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

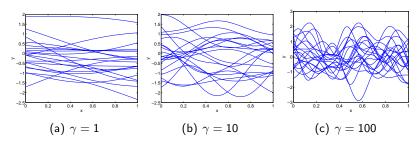


Figure 7: Varying hyper-parameters in an RBF covariance varies the smoothness of the function.

Optimising hyper-parameters

Making predictions

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

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

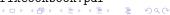
▶ And then use standard results for Gaussian conditionals:

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

where

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

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



Noise-free example

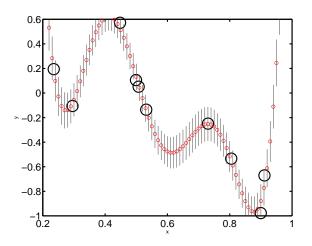


Figure 8 : $\mu_* \pm \sigma_*$ for a noise-free GP at lots of test points

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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▶ 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

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

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

Example with noise

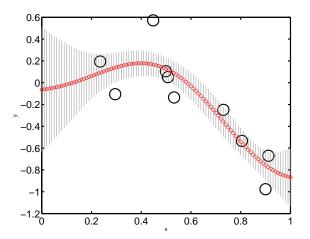


Figure 9 : $\mu_* \pm \sigma_*$ at lots of test points when observation noise is included.

Lecture 3: Application: Touchscreen typing

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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

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- Occlusion of target by finger
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- Small targets
- ▶ Demo: http://bit.ly/1nBws97
- Quite a bit of work in this area:
 - Add some

Background 2: All users are different

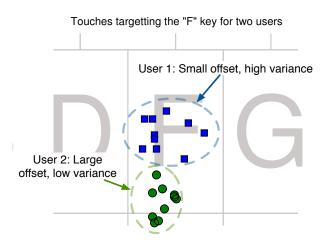


Figure 10: Touches recorded by two users aiming for the 'F' key. User 2 has high bias and low variance, user 1 has low bias and high variance.

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 → HELLO'

- 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!

- There is a lot of uncertainty present in touch (bias and variance)
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- 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.



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.



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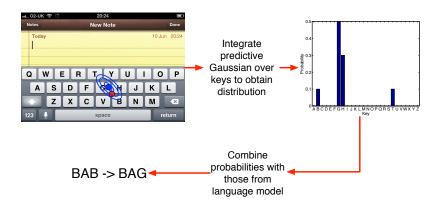


Figure 12: The complete system

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

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- ▶ 10 participants, each did 3× 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

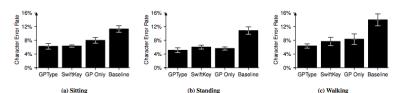


Figure 4. Character error rates for the two keyboards we evaluated, separated by mobility condition (Study 2). Plots show mean and standard error across all participants. The baseline method represents the literal keys touched, while GP Only shows the keys hit after the mean GP offset is applied.

Figure 13: Results of GPType experiment

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

Conclusions

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- More info:
 - http://www.youtube.com/watch?v=11QI5gV5174
 - http://pokristensson.com/pubs/WeirEtAlCHI2014.pdf
 - Acknowledgements: Daryl Weir, Per Ola Kristensson, Keith Vertanen, Henning Pohl



Lecture 4: Application: Clinical Ratings

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Clinicians disagree in AandE