Gaussian Process Classification, Approximations and Other GP Models

COMP9418 — Advanced Topics in Statistical Machine Learning

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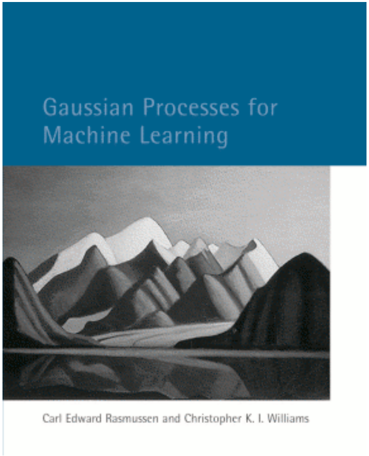
Acknowledgements



Carl Edward Rasmussen and Christopher K. I. Williams

All chapters available online along with software and datasets:
`http://www.gaussianprocess.org/gpml`

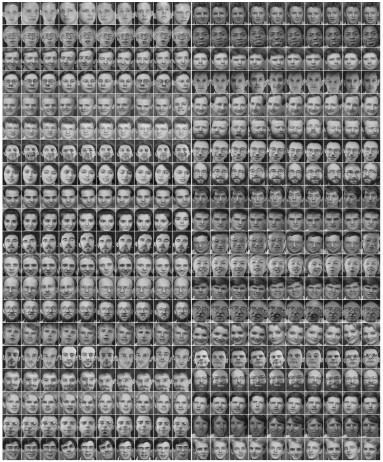
Aims

This lecture will allow you to understand and apply Gaussian process classification and approximations methods to large datasets. Following it you should be to:

- Understand and apply Gaussian process binary classification with posterior inference via the Laplace approximation.
- Understand and apply scalable approaches to Gaussian process regression from a unifying probabilistic framework.
- Understand other models with Gaussian process priors and non-linear likelihoods and their applications such as multi-task learning (MTGP) and latent-variable models (GPLVM).

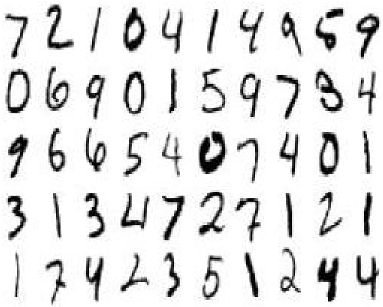
Classification Problems

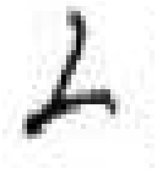
Facial Recognition


Examples of faces and their identity.

what is his/her identity?

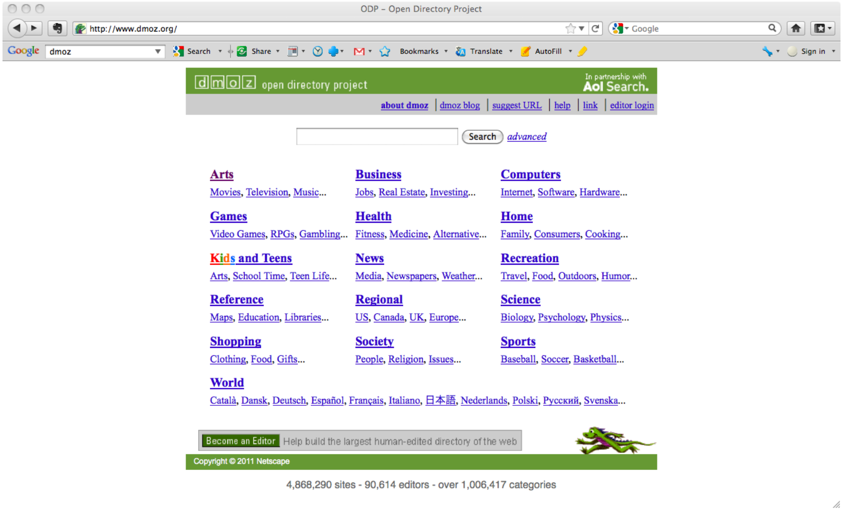
Classification Problems
Handwritten Digit Recognition


Examples of images and their corresponding digit.


What is the number in the image?

Classification Problems

Supervised Document Classification


ODP – Open Directory Project
http://www.dmoz.org/
Google
dmoz
Search
Share
Bookmarks
Translate
AutoFill
Sign in
dmoz open directory project
In partnership with Aol Search.
about dmoz | dmoz blog | suggest URL | help | link | editor login
Search
advanced

Arts
Movies, Television, Music...

Business
Jobs, Real Estate, Investing...

Computers
Internet, Software, Hardware...

Games
Video Games, RPGs, Gambling...

Health
Fitness, Medicine, Alternative...

Home
Family, Consumers, Cooking...

Kids and Teens
Arts, School Time, Teen Life...

News
Media, Newspapers, Weather...

Recreation
Travel, Food, Outdoors, Humor...

Reference
Maps, Education, Libraries...

Regional
US, Canada, UK, Europe...

Science
Biology, Psychology, Physics...

Shopping
Clothing, Food, Gifts...

Society
People, Religion, Issues...

Sports
Baseball, Soccer, Basketball...

World
Català, Dansk, Deutsch, Español, Français, Italiano, 日本語, Nederlands, Polski, Русский, Svenska...

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4,868,290 sites - 90,614 editors - over 1,006,417 categories

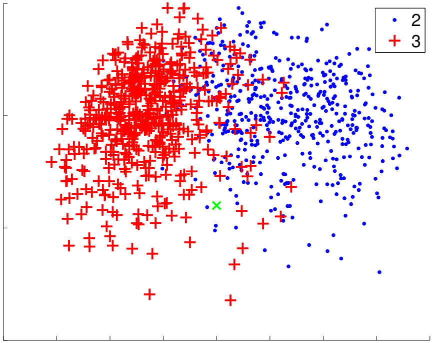
The Classification Problem

Problem Definition

In all previous problems we are dealing with **discrete** targets.

Given a set of input-output pairs $\mathcal{D} = \{\mathbf{x}^{(n)}, y^{(n)}\}_{n=1}^{N}$ where $\mathbf{x}$ is a D-dimensional feature vector and $y \in \{\mathcal{C}_1, \ldots, \mathcal{C}_M\}$.

Goal: Learn a mapping $f(\mathbf{x}) : \mathbf{x} \rightarrow y$ in order to make predictions at unseen datapoints $\mathbf{x}^*$.



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Some Concepts

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- Binary classification: $\{0, 1\}$, $\{-1, 1\}$
- Multiclass classification: 1-of-M encoding
  e.g. $y = (0, 0, 0, 1, 0)^T$ denoting the instance belongs to class 4 (out of $M = 5$ classes)

Discriminative vs Generative Approaches

Generative

Model the joint $p(\mathbf{x}, y)$ via models for $p(\mathbf{x}|y)$ and $p(y)$.

Predictions $p(y|\mathbf{x})$ via Bayes rule

+ Amenable to incorporation of prior knowledge

– Indirect approach

Discriminative

Model $p(y|\mathbf{x})$ directly.

– Difficult to incorporate prior information

+ Focus on the task at hand

Decision Theory for Classification

A probabilistic classifier provides an elegant framework for decision theory:

Suppose that we have a predictive probability $p(y = c|\mathbf{x})$

Let $\underline{L}(c, c')$ be the loss incurred by making a decision c' when the true class is c.

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For the case of the 0-1 loss (a unit penalty is paid for a misclassification), the optimal decision maximizes $p(c|\mathbf{x}_*)$

This optimal classifier is know as **Bayes classifier**.

Outline

Linear Models for Classification

Data : $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$, $\mathbf{x} \in \mathbb{R}^{D}$, $y \in \{-1, +1\}$

Input : $(\mathbf{X})_{D \times N}$, Targets: $(\mathbf{y})_{N \times 1}$

Goal : Make predictions at $\mathbf{x}_*$

Model : $p(y = +1|\mathbf{X}, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x})$

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- Logistic Regression $\sigma(z) = \dfrac{1}{1 + \exp(-z)}$

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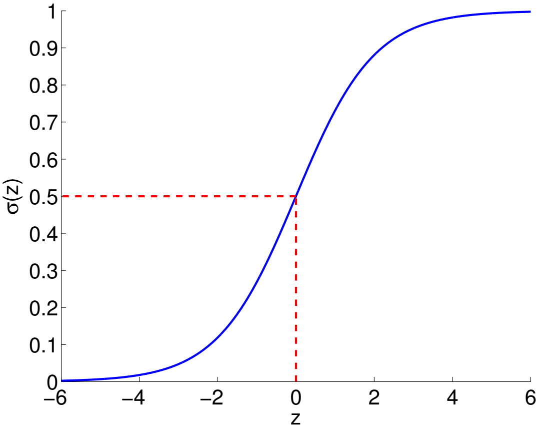
Two popular approaches:

- Logistic Regression $\sigma(z) = \dfrac{1}{1 + \exp(-z)}$
- Probit Regression: $\sigma(z) = \int_{-\infty}^{z} \mathcal{N}(x|0, 1) dx$

Logistic Regression
The Logit (or Logistic Sigmoid) Function



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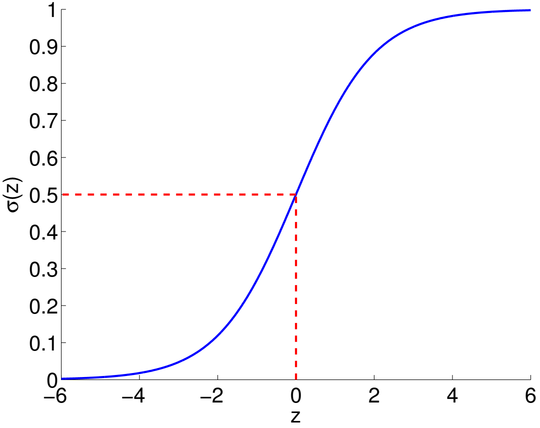

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How do we learn the weights?

MAP Approach

As in Bayesian linear regression we can use the prior:

$$\mathbf{w} \sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\Sigma}_w).$$

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However, the full posterior does not have a simple analytical form. We write down the un-normalized log-posterior:

$$\mathcal{L}^{\text{MAP}} = \sum_{i=1}^{N} \log \sigma(y^{(i)} f_i) - \frac{1}{2} \mathbf{w}^T \mathbf{\Sigma}_w^{-1} \mathbf{w},$$

Where $f_i \overset{\text{def}}{=} \mathbf{w}^T \mathbf{x}_i$.

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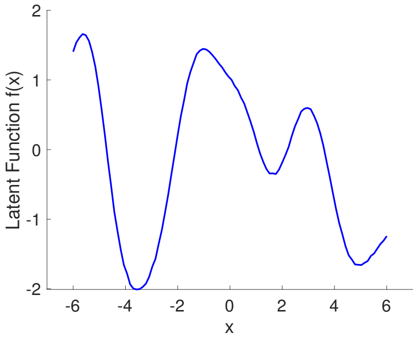
Multi-class case is addressed with a softmax function.

Gaussian Process Classification (GPC)

Binary Classification

Discriminative approach:

1. Place prior over the latent functions $f(\mathbf{x})$



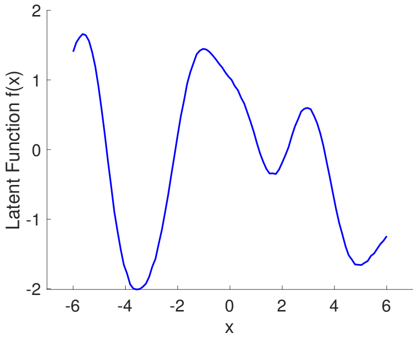
Sample from a GP

Gaussian Process Classification (GPC)

Binary Classification

Discriminative approach:

1. Place prior over the latent functions $f(\mathbf{x})$
2. Squash this through a sigmoid function: $p(y=+1|\mathbf{x}) = \sigma(f(\mathbf{x}))$



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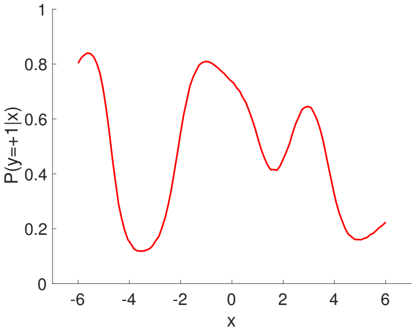

$\sigma(f(x)) = \frac{1}{1+e^{-f(x)}}$

GPC Model

Data : $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$, $\mathbf{x} \in \mathbb{R}^{D}$, $y \in \{-1, +1\}$

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Prior : $f \sim \mathcal{GP}\left(0, \kappa(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta})\right) \rightarrow p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K})$,

Likelihood : $p(y = +1|f) = \sigma(f(x)) \overset{\text{iid}}{\rightarrow} p(\mathbf{y}|\mathbf{f}) = \prod_{i=1}^{N} \sigma(y^{(i)} f_i)$,

- $(\mathbf{f})_{N \times 1}$ vector of latent variables
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Posterior $p(\mathbf{f}|\mathbf{X}, \mathbf{y}) \propto p(\mathbf{f}|\mathbf{X}) p(\mathbf{y}|\mathbf{f})$ analytically intractable

- Due to non-Gaussian likelihood $p(\mathbf{y}|\mathbf{f})$

Need to resort to approximations

GPC Inference

1. Compute predictive distribution of latent functions:

$$p(f_*|\mathbf{X}, \mathbf{y}, \mathbf{x}_*) = \int p(f_*|\mathbf{X}, \mathbf{x}_*, \mathbf{f}) p(\mathbf{f}|\mathbf{X}, \mathbf{y}) d\mathbf{f}$$

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2. Compute probabilistic predictions:

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   - Analytic solution for the probit model
   - Require numerical approximations (1D) integral for other sigmoid functions

The Laplace Approximation

Idea: Find a Gaussian approximation to $p(z) = \frac{1}{Z} f(z)$, where Z is unknown. We centre the Gaussian approximation at the mode of $p(z)$.

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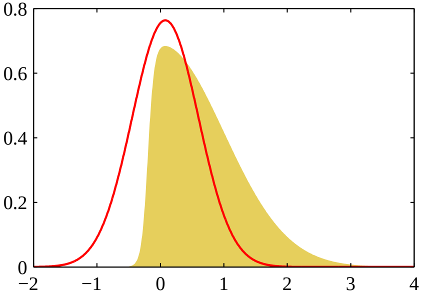

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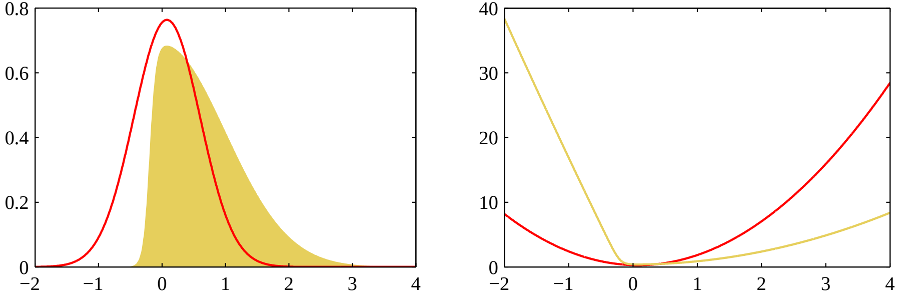

Figures by Christopher M. Bishop (MLPR, 2006)

Left : $p(z) \propto \exp(-z^2/2)\sigma(20z + 4)$ and corresponding Gaussian approximation.

Right : Negative logarithms of the corresponding curves.

The Laplace Approximation to the GP Binary Classifier

Gaussian approximation

$$p(\mathbf{f}|\mathbf{X}, \mathbf{y}, \boldsymbol{\theta}) \approx \mathcal{N}(\mathbf{f}|\hat{\mathbf{f}}, A^{-1})$$

where: $\hat{\mathbf{f}} = \text{argmax}_{\mathbf{f}}\, p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}) = \text{argmax}_{\mathbf{f}}\;\; p(\mathbf{y}|\mathbf{f}, \boldsymbol{\theta}) p(\mathbf{f}|\mathbf{X}, \boldsymbol{\theta})$ and A is the Hessian of the negative log-posterior evaluated at $\hat{\mathbf{f}}$.

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Hence we focus on the maximization of:

$$\psi(\mathbf{f}) = \log p(\mathbf{y}|\mathbf{f}) - \frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f} - \frac{1}{2}\log|\mathbf{K}| - \frac{N}{2}\log 2\pi$$

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$$\mathbf{f}^{\text{new}} = (\mathbf{W} + \mathbf{K}^{-1})^{-1}\left(\frac{\partial \log p(\mathbf{y}|\mathbf{f})}{\partial \mathbf{f}} + \mathbf{W}\mathbf{f}\right)$$

with $\mathbf{W}_{pq} = \dfrac{\partial^2 \log p(\mathbf{y}|\mathbf{f})}{\partial f_p \partial f_q}$.

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Constraint on A? What does this imply?

The Lapace Approximation to GPC

Convergence and Uniqueness:

- Note that $\mathbf{W}$ is a diagonal matrix due to iid assumption
- for concave likelihood functions the un-normalized log posterior has a unique maximum

Once we have found the maximum posterior $\hat{\mathbf{f}}$ by using the above iteration we can show that:

$$p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}) \approx \mathcal{N}(\mathbf{f}|\hat{\mathbf{f}}, (\mathbf{W} + \mathbf{K}^{-1})^{-1}).$$

When is this approximation a good/bad idea?

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When is this approximation a good/bad idea?

- Better when N is large
- Only model aspects of distribution at a specific value
- Essentially uncontrolled (Hessian may be poor approximation to true shape of the posterior)

Posterior and Predictive Distributions

Recalling the posterior distribution:

$$p(f_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) = \int p(f_* | \mathbf{X}, \mathbf{x}_*, \mathbf{f}) p(\mathbf{f} | \mathbf{X}, \mathbf{y}) d\mathbf{f}$$

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Hence, under Laplace approximation:

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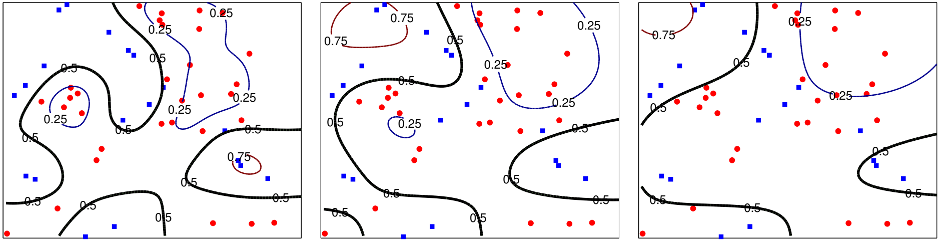
- They provide the same prediction when concerned with most probable classification
- Full distribution is required if we are concerned with confidence in the predictions (e.g. reject options)

Marginal Likelihood and hyper-parameter learning

We can also apply the Laplace approximation to the marginal likelihood:

$$\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) \approx -\frac{1}{2}\log|\mathbf{KW} + \mathbf{I}| - \frac{1}{2}\hat{\mathbf{f}}^T\mathbf{K}^{-1}\hat{\mathbf{f}} + \log p(\mathbf{y}|\hat{\mathbf{f}})$$

Predictive probability as a function of the length-scale $\ell = 0.1, 0.2, 0.3$:



Do we spend too much effort in modeling f?

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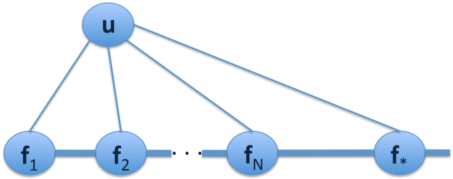

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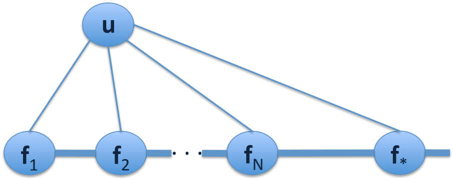

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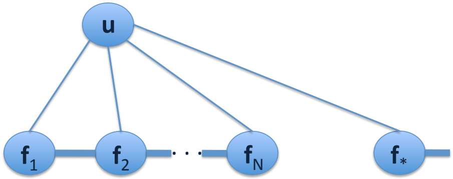

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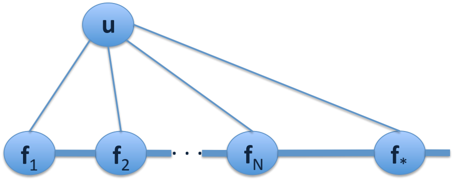

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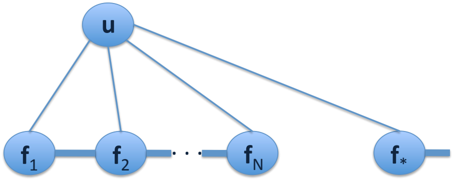

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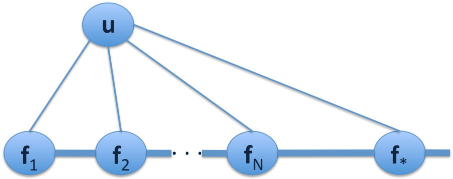

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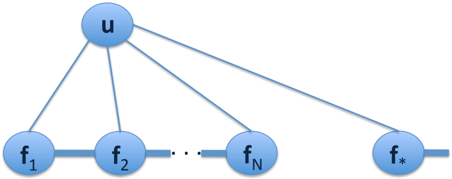

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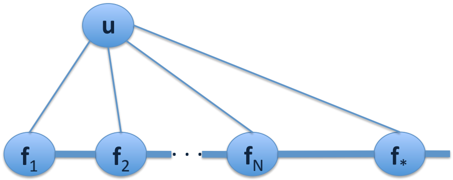

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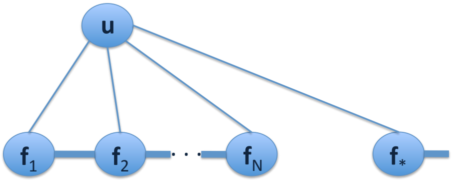

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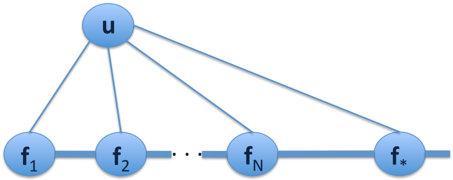

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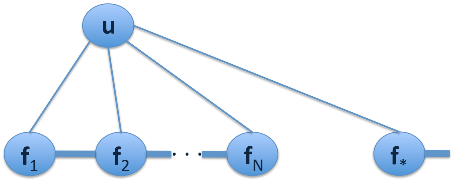

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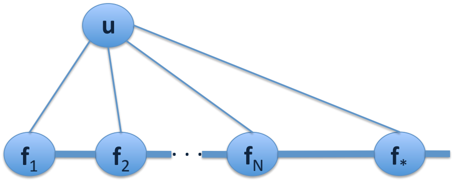

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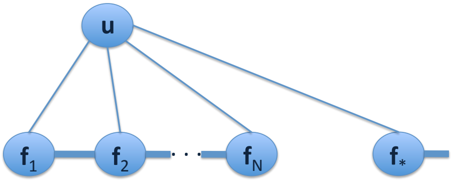

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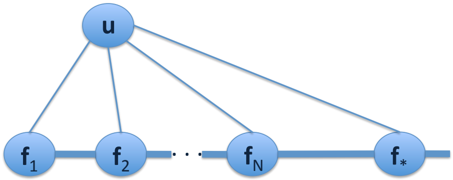

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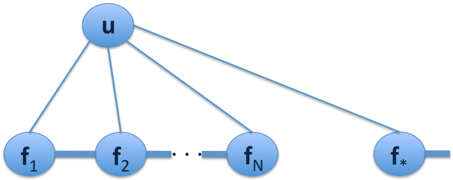

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Most approximation methods can be defined by:

- Different specifications of these conditionals.
- Different $\mathbf{Z}$: Subset of training/test points, new $\mathbf{x}$ points

Subset of Regressors (SR)

It can be shown that the mean GP predictor can be obtained by assuming:

$$\begin{aligned} \text{Prior} &: \boldsymbol{\alpha} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}^{-1}) \\ \text{Model} &: f(\mathbf{x}_*) = \textstyle\sum_{i=1}^{N} \alpha_i k(\mathbf{x}_*, \mathbf{x}^{(i)}) \end{aligned}$$

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where $\boldsymbol{\Sigma} = \mathbf{K}_{\text{zx}}\mathbf{K}_{\text{xz}} + \sigma_n^2\mathbf{K}_{\text{zz}}$.

- This method corresponds to a degenerate GP prior

Subset of Regressors (SR)

It can be shown that the mean GP predictor can be obtained by assuming:

Prior : $\boldsymbol{\alpha} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}^{-1})$

Model : $f(\mathbf{x}_*) = \sum_{i=1}^{N} \alpha_i k(\mathbf{x}_*, \mathbf{x}^{(i)})$

We can truncate the number of regressors needed:

$$f_{\mathrm{SR}}(\mathbf{x}_*) = \mathbf{k}_*^T \boldsymbol{\alpha}_{\mathrm{z}} \text{ with } \boldsymbol{\alpha}_{\mathrm{z}} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathrm{zz}}^{-1})$$

This implies that there is a deterministic relation between $\mathbf{f}_*$ and $\mathbf{u}$:

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- This method corresponds to a degenerate GP prior
- Complexity: $\mathcal{O}(M^2N)$ initially and $\mathcal{O}(M)$ and $\mathcal{O}(M^2)$ per test predictive mean and variance.

Projected Processes (PP)

$$q_{\mathrm{PP}}(\mathbf{f}|\mathbf{u}) = \mathcal{N}(\mathbf{K}_{\mathrm{xz}}\mathbf{K}_{\mathrm{zz}}^{-1}\mathbf{u}, \mathbf{0}) \quad q_{\mathrm{PP}}(\mathbf{f}_*|\mathbf{u}) = p(\mathbf{f}_*|\mathbf{u})$$

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- As in SR, it imposes a deterministic training conditional but (unlike SR) it uses the exact test conditional.
- Same predictive mean as SR but variances are never smaller
- However, this definition implies that the covariances for training cases and test cases are computed differently and therefore this method does not correspond to a (consistent) GP.

FITC, PITC and BCM

FITC	: Fully independent training conditionals
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- PITC uses block diagonal covariance to improve the approximation
- BCM is the same as PITC where the choice of inducing variables depend on the test points, i.e. transductive setting
  - However, note that transduction cannot occur in exact GPs
  - Drawback regarding complexity of transductive models?
  - The choice of $\mathbf{u}$ should not be dictated only by the test points

Sparse GPs (Snelson and Ghahramani, 2006)

- Same as FITC but the inducing inputs do not belong to the training or test sets
- Both the locations of the input points and the values of the hyper-parameters are “learned” by optimization of the approximate marginal likelihood.

GP Approximations: Final Remarks

- The order of computational complexity is identical for all methods (except SD)
- Hence, there is no "excuse for gross approximations"
- Inconclusive experiments on real datasets (See e.g. Rassmussen and Williams, 2006)
- Similar methods for GP classification but we also need to deal with non-Gaussian likelihoods (e.g. using Laplace)
  - Derivatives of the marginal likelihood can get complicated

Multi-task Learning (MTL)

- General idea:
  - Sharing information across tasks (Caruana, 1997)
  - Very little data on test task
  - Exam score prediction, compiler performance prediction, robot inverse dynamics, multi-topic text categorisation, collaborative filtering, multi-level modelling

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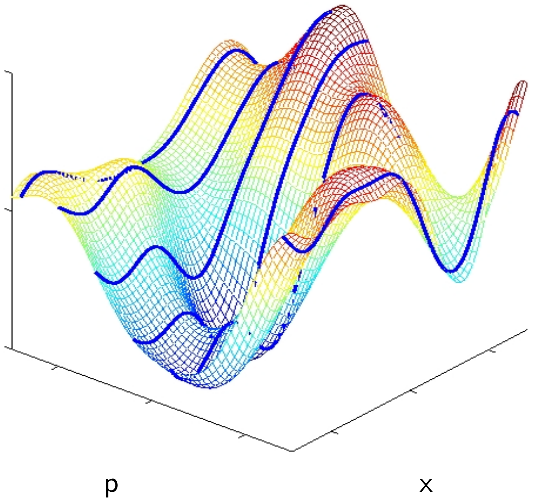
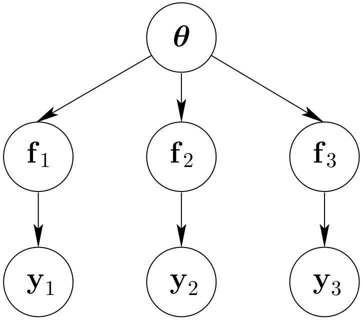
  - Exam score prediction, compiler performance prediction, robot inverse dynamics, multi-topic text categorisation, collaborative filtering, multi-level modelling
- Assuming task relatedness can be detrimental (Caruana, 1997; Baxter, 2000)
- Task descriptors may be available (Bonilla et al, AISTATS 2007)
- Tasks descriptors unavailable or difficult to define correctly (Bonilla et al, NIPS 2008)
  - e.g. Compiler performance prediction: code features, responses

Multi-task GP: Illustration



Sample functions for different values of tasks (on *p* axis) are correlated (cf **independent** draws over sample functions)

Inter-task Tying by Hyper-parameter Sharing


$$\begin{tikzcd} & \boldsymbol{\theta} \arrow[dl] \arrow[d] \arrow[dr] & \\ \mathbf{f}_1 \arrow[d] & \mathbf{f}_2 \arrow[d] & \mathbf{f}_3 \arrow[d] \\ \mathbf{y}_1 & \mathbf{y}_2 & \mathbf{y}_3 \end{tikzcd}$$

Other approaches

- Block diagonal covariance matrix, and each of the P blocks is induced from the same kernel function (Minka and Picard, 1999; Lawrence and Platt, 2004; Yu et al, 2005; Schwaighofer et al, 2005)

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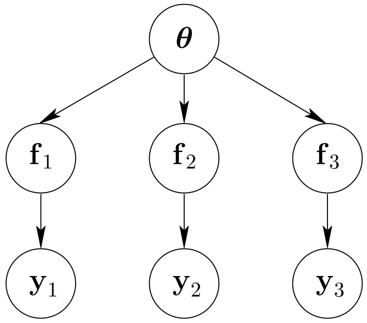

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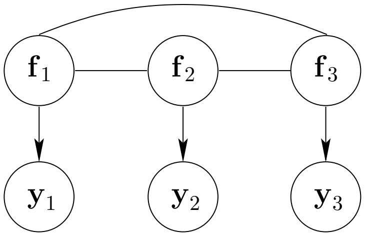

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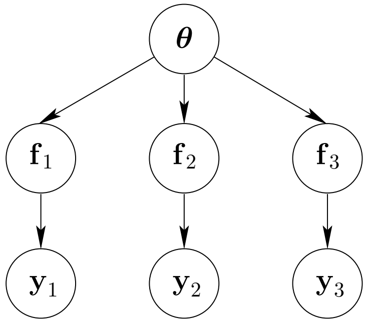

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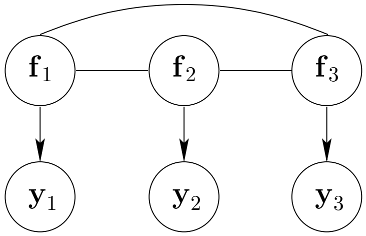

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- Block diagonal covariance matrix, and each of the P blocks is induced from the same kernel function (Minka and Picard, 1999; Lawrence and Platt, 2004; Yu et al, 2005; Schwaighofer et al, 2005)
- Multi-task GP: Observations on one task affect predictions on the others

Multi-task GP (MTGP)

We place a (zero mean) GP prior over the latent functions $\{f_\ell\}$:

The Model

$$\langle f_\ell(\mathbf{x}) f_m(\mathbf{x}') \rangle = K^f_{\ell m} k^x(\mathbf{x}, \mathbf{x}') \qquad y_{i\ell} \sim \mathcal{N}(f_\ell(\mathbf{x}^{(i)}), \sigma^2_\ell),$$

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Correlations between tasks modelled directly via K^f

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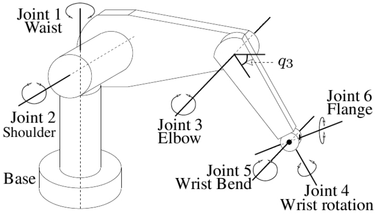
- Mixture: All functions are independent except for one, which is a mixed version of the others. Effective for transferring to a new task:

$$K^f = \begin{pmatrix} I & \boldsymbol{\pi} \\ \boldsymbol{\pi}^{\mathsf{T}} & \boldsymbol{\pi}^{\mathsf{T}}\boldsymbol{\pi} \end{pmatrix},$$

where $\boldsymbol{\pi}$ are mixing proportions, and may depend on task descriptors.

Learning Robot Inverse Dynamics (Chai et al, NIPS 2009)



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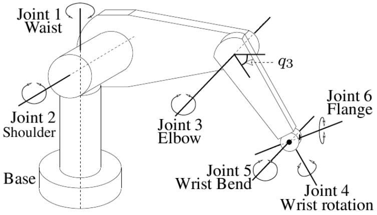

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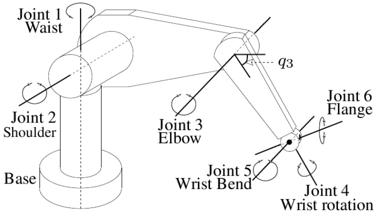

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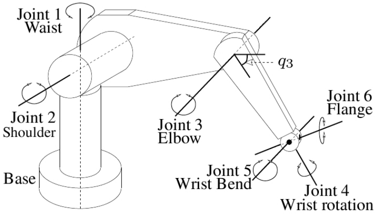

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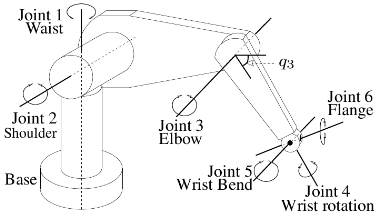

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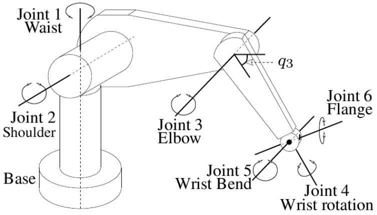

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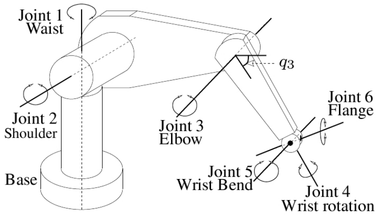

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The MTGP model matches the correlations between torque functions

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- GP models for pose estimation: `http://grail.cs.washington.edu/projects/styleik`

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- GPLVM predictive distribution is used in objective function to find new poses given the constraints.

Pose Estimation Movies

From `http://grail.cs.washington.edu/projects/styleik`

Style Pitch

Style Track

Pose Track

Image Pose Basketball

Image Pose Baseball

Interpolation

Conclusions

- GPs as flexible non-parameteric Bayesian technique for regression, classification and other machine learning problems.
- The covariance function is a crucial component in GPs.
- Analytic solutions for standard regression setting and approximate inference for classification.
- Computational issues dealt with through the idea of inducing variables and a single unifying probabilistic framework.
- Dealing with non-standard settings, e.g. preference learning and multi-task learning.
- Reading:
  - Rasmussen & Williams (GPML, 2006): Ch. 3 (except sec 3.5, 3.6), Ch. 8
  - [Strongly recommended] Quiñonero-Candela and Rasmussen (A Unifying View of Sparse Approximate Gaussian Process Regression, JMLR, 2005)