# Gaussian Processes 

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Machine Learning Summer School

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## The Book



Carl Edward Rasmussen and Christopher K. I. Williams

## Carl Edward Rasmussen and Christopher K. I. Williams

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

## The Prediction Problem

Learn mapping $\mathbf{x} \rightarrow \mathbf{f}(\mathbf{x})$ from observations $\left\{\left(\mathbf{x}_{i}, y_{i}\right)\right\}_{i=1}^{N}$.


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- Flexibility v generalization
- What basis functions? How many?


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We can address these issues in a principled way with Gaussian Processes

## Demo



- Smooth functions
- Closeness in input space $\rightarrow$ closeness in output space


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- Hyperparameter learning
- Many standard regression models are special cases of GPs
- GP models also applicable to non-regression settings


## Outline

(1) The Gaussian Distribution
(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression
(4) Gaussian Processes for Classification
(5) Approximations for Large Datasets
(6) Current Research
(7) Conclusions

## (1) The Gaussian Distribution

(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression

4 Gaussian Processes for Classification
(5) Approximations for Large Datasets
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## The Gaussian Distribution

## 1D Example

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$p(x)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(-\frac{1}{2 \sigma^{2}}(x-\mu)^{2}\right)$

$F(x)=\int_{-\infty}^{x} \mathcal{N}\left(z \mid \mu, \sigma^{2}\right) d z$

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$F(x)=\int_{-\infty}^{x} \mathcal{N}\left(z \mid \mu, \sigma^{2}\right) d z$

In general: $p(x)=\mathcal{N}(x \mid \mu, \Sigma)=\frac{1}{|2 \pi \Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}(x-\mu)^{\top} \Sigma^{-1}(x-\mu)\right)$

## The Gaussian Distribution <br> 2D Example



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## 2D Example




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## The Gaussian Distribution

## 2D Example



Marginal


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\binom{\mathrm{x}_{1}}{\mathrm{x}_{2}} \sim \mathcal{N}\left(\left[\begin{array}{l}
\mu_{1} \\
\mu_{2}
\end{array}\right],\left[\begin{array}{ll}
\boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\
\boldsymbol{\Sigma}_{12}^{\top} & \boldsymbol{\Sigma}_{22}
\end{array}\right]\right)
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## The Gaussian Distribution

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& \mathbf{x}_{1} \sim \mathcal{N}\left(\mathbf{x}_{1} \mid \mu_{1}, \boldsymbol{\Sigma}_{11}\right)
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## The Gaussian Distribution

## 2D Example


$p\left(\chi_{1}, \chi_{2}\right) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
Joint

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\mathbf{x}_{1} & \sim \mathcal{N}\left(\mathrm{x}_{1} \mid \mu_{1}, \Sigma_{11}\right) \\
\mathbf{x}_{1} \mid \mathbf{x}_{2} & \sim \mathcal{N}\left(\mathbf{x}_{1} \mid \mu_{1}+\Sigma_{12} \Sigma_{22}^{-1}\left(\mathbf{x}_{2}-\mu_{2}\right), \Sigma_{11}-\Sigma_{12} \Sigma_{22}^{-1} \Sigma_{12}^{\top}\right)
\end{aligned}
$$

## The Gaussian Distribution

Covariance and Precision Matrices

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p(\mathbf{x})=\mathcal{N}(\mathbf{x} \mid \mu, \Sigma)=\frac{1}{|2 \pi \Sigma|^{1 / 2}} \exp \left(-\frac{1}{2}(\mathbf{x}-\mu)^{\top} \Sigma^{-1}(\mathbf{x}-\mu)\right)
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- An entry $\boldsymbol{\Sigma}_{\mathfrak{i j}}=0$ indicates that the variables $\mathfrak{i}$ and $\mathfrak{j}$ are marginally independent given all the other variables.


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- An entry $\boldsymbol{\Sigma}_{\mathfrak{i j}}^{-1}=0$ indicates that the variables $i$ and $j$ are conditionally independent given all the other variables.
- An entry $\boldsymbol{\Sigma}_{i j}=0$ indicates that the variables $i$ and $j$ are marginally independent given all the other variables.
- Marginalizing out a variable leaves $\boldsymbol{\Sigma}$ unchanged but changes $\boldsymbol{\Sigma}^{-1}$.
- This is crucial when parameterizing a Gaussian process.


## Gaussian Quiz

## (1) The Gaussian Distribution

(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression

44 Gaussian Processes for Classification
(5) Approximations for Large Datasets
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## The Standard Linear Regression Model

Notation and Settings

$$
\begin{aligned}
\text { Data } & : \mathcal{D}=\left\{\left(\mathbf{x}_{i}, y_{i}\right)\right\}_{i=1}^{N}, \mathbf{x} \in \mathbb{R}^{\mathrm{D}}, \mathbf{y} \in \mathbb{R} \\
\text { Input } & :(\mathbf{X})_{\mathrm{D} \times N}, \text { Targets: }(\mathbf{y})_{\mathrm{N} \times 1} \\
\text { Goal } & : \mathbf{x} \xrightarrow{\mathbf{f ( x )}} \mathbf{y}
\end{aligned}
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Input: $(\mathbf{X})_{\mathrm{D} \times \mathrm{N}}$, Targets: $(\mathbf{y})_{\mathrm{N} \times 1}$
Goal : $\mathbf{x} \xrightarrow{\mathbf{f}(\mathbf{x})} \mathbf{y}$
Model $\quad \mathrm{f}(\mathrm{x})=\sum_{\mathrm{i}=1}^{\mathrm{D}} w_{\mathrm{i}} x_{\mathrm{i}} \quad=\mathrm{w}^{\top} \mathrm{x}$
Noise $\quad y=f(x)+\eta \quad$ with $\eta \sim \mathcal{N}\left(\eta \mid 0, \sigma^{2}\right)$
Likelihood $y \mid f(x) \sim \mathcal{N}\left(y \mid f(x), \sigma^{2}\right)=\mathcal{N}\left(y \mid w^{\top} x, \sigma^{2}\right)$

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Thus, the data-likelihood is given by:

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\begin{aligned}
p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) & =\prod_{\mathfrak{i}=1}^{N} p\left(y_{i} \mid \mathbf{x}_{i}, \mathbf{w}\right)=\prod_{i=1}^{N} \mathcal{N}\left(y_{i} \mid \mathbf{w}^{\top} \mathbf{x}_{i}, \sigma^{2}\right) \\
& =\mathcal{N}\left(\mathbf{y} \mid \mathbf{X}^{\top} \mathbf{w}, \sigma^{2} \mathbf{I}\right)
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We need do to inference on $\mathbf{w}$.

## Bayesian Linear Regression

## Posterior Distribution

Consider a zero-mean Gaussian prior over the weights:

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\mathbf{w} \sim \mathcal{N}\left(\mathbf{w} \mid \mathbf{0}, \boldsymbol{\Sigma}_{w}\right)
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where $\overline{\mathbf{w}}=\frac{1}{\sigma^{2}} \mathbf{A}^{-1} \mathbf{X y}$, and $\mathbf{A}=\left(\frac{1}{\sigma^{2}} \mathbf{X} \mathbf{X}^{\top}+\boldsymbol{\Sigma}_{w}^{-1}\right)$.

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- Mean of posterior is equal to its mode
- MAP solution (non-Bayesian): negative log prior as penalty term
- This penalized maximum likelihood is known as ridge regression
- Consider $\boldsymbol{\Sigma}_{w}=\lambda \mathbf{I}$ Then:

$$
\overline{\mathbf{w}}=\left(\mathbf{X} \mathbf{X}^{\top}+\frac{1}{\lambda} \sigma^{2} \mathbf{I}\right)^{-1} \mathbf{X} \mathbf{y}
$$

## Bayesian Linear Regression

## Predictive Distribution

We are interested in making predictions at a new test point $\mathbf{x}_{*}$

- In fact we obtain the predictive distribution by averaging over all possible parameter values (weighted by their posterior probabilities):

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p\left(f_{*} \mid \mathbf{x}_{*}, \mathbf{X}, \mathbf{y}\right)=\int p\left(f_{*} \mid \mathbf{x}_{*}, \mathbf{w}\right) p(\mathbf{w} \mid \mathbf{X}, \mathbf{y}) \mathrm{d} \mathbf{w}=\mathcal{N}\left(\mathbf{f}_{*} \mid \mathbf{x}_{*}^{\top} \overline{\mathbf{w}}, \mathbf{x}_{*}^{\top} \mathbf{A}^{-1} \mathbf{x}_{*}\right)
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- Predictive mean: linear combination of weights' posterior mean
- Predictive variance: grows with the magnitude of the test point


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$$

- Predictive mean: linear combination of weights' posterior mean
- Predictive variance: grows with the magnitude of the test point
- Point predictions: Need to consider the expected loss (or risk):

$$
y_{\text {opt }}=\underset{y_{\text {pred }}}{\operatorname{argmin}} \int \mathcal{L}\left(f_{*}, y_{\text {pred }}\right) p\left(f_{*} \mid \mathbf{x}_{*}, \mathbf{X}, \mathbf{y}\right) \mathrm{df}_{*}
$$

- e.g. Square loss $\mathcal{L}=\left(y_{\text {pred }}-f_{*}\right)^{2}$
- c.f. Empirical risk minimization (ERM)


## Bayesian Linear Regression Example



## Bayesian Linear Regression Example



## Bayesian Linear Regression Example


Prior Weights



## Bayesian Linear Regression Example




Observed Data


Likelihood

## Bayesian Linear Regression Example



Prior Weights


Likelihood


Predictive Distribution


Posterior Weights

## Non-linear Feature Spaces

- Consider the model $f(\mathbf{x})=\sum_{i=1}^{\mathrm{D}^{\prime}} w_{i} \phi_{\mathfrak{i}}(\mathbf{x})=\mathbf{w}^{\top} \boldsymbol{\phi}(\mathbf{x})$
- Each $\phi_{i}(x)$ is a (non-linear) feature on $x$, e.g. $x_{1}, x_{2}, x_{1}^{2}, x_{2}^{2}, x_{1} x_{2} \ldots$
- We have a non-linear mapping but a linear-in-the-parameters model
- The number of these features can be very large, i.e. $\mathrm{D}^{\prime} \gg \mathrm{D}$


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- All the Bayesian analysis is similar to the standard linear model:

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p\left(f_{*} \mid \mathbf{x}_{*}, \mathbf{X}, \mathbf{y}\right)=\mathcal{N}\left(f_{*} \mid \sigma^{-2} \boldsymbol{\phi}_{*}^{\top} \mathbf{A}^{-1} \boldsymbol{\Phi} \mathbf{y}, \boldsymbol{\phi}_{*}^{\top} \mathbf{A}^{-1} \boldsymbol{\phi}_{*}\right)
$$

where: $\boldsymbol{\phi}_{*}=\boldsymbol{\phi}\left(\mathbf{x}_{*}\right), \boldsymbol{\Phi}=\boldsymbol{\Phi}(\mathbf{X})$, and $\mathbf{A}=\left(\frac{1}{\sigma^{2}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\top}+\boldsymbol{\Sigma}_{w}^{-1}\right)$

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- Note we need to invert $\mathbf{A}$ of ? dimensions.


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\mathfrak{p}\left(\mathbf{f}_{*} \mid \mathbf{x}_{*}, \mathbf{X}, \mathbf{y}\right)=\mathcal{N}\left(\mathbf{f}_{*} \mid \sigma^{-2} \boldsymbol{\phi}_{*}^{\top} \mathbf{A}^{-1} \boldsymbol{\Phi} \mathbf{y}, \boldsymbol{\phi}_{*}^{\top} \mathbf{A}^{-1} \boldsymbol{\phi}_{*}\right)
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where: $\boldsymbol{\phi}_{*}=\boldsymbol{\phi}\left(\mathrm{x}_{*}\right), \boldsymbol{\Phi}=\boldsymbol{\Phi}(\mathbf{X})$, and $\mathbf{A}=\left(\frac{1}{\sigma^{2}} \boldsymbol{\Phi} \boldsymbol{\Phi}^{\top}+\boldsymbol{\Sigma}_{w}^{-1}\right)$

- Note we need to invert A of ? dimensions.
- We can rewrite the predictive distribution as:

$$
p\left(\mathbf{f}_{*} \mid \mathbf{x}_{*}, \mathbf{X}, \mathbf{y}\right)=\mathcal{N}\left(\mathbf{f}_{*} \mid \mathbf{k}_{*}^{\top} \widetilde{\mathbf{K}}^{-1} \mathbf{y}, \mathrm{k}_{\star *}-\mathbf{k}_{*}^{\top} \widetilde{\mathbf{K}}^{-1} \mathbf{k}_{*}\right)
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where $\mathbf{k}_{*}=\boldsymbol{\Phi}^{\top} \boldsymbol{\Sigma}_{\mathcal{w}} \boldsymbol{\Phi}_{*}, \mathrm{k}_{\star \star}=\boldsymbol{\phi}_{*}^{\top} \boldsymbol{\Sigma}_{w} \boldsymbol{\Phi}_{*}$, and $\widetilde{\mathbf{K}}=\boldsymbol{\Phi}^{\top} \boldsymbol{\Sigma}_{\mathcal{w}} \boldsymbol{\Phi}+\sigma^{2} \mathbf{I}$

## Non-linear Feature Spaces

- Consider the model $f(\mathbf{x})=\sum_{i=1}^{\mathrm{D}^{\prime}} w_{i} \phi_{\mathfrak{i}}(\mathbf{x})=\mathbf{w}^{\top} \boldsymbol{\phi}(\mathbf{x})$
- Each $\phi_{i}(\mathbf{x})$ is a (non-linear) feature on x , e.g. $\mathrm{x}_{1}, x_{2}, x_{1}^{2}, x_{2}^{2}, x_{1} x_{2} \ldots$
- We have a non-linear mapping but a linear-in-the-parameters model
- The number of these features can be very large, i.e. $\mathrm{D}^{\prime} \gg \mathrm{D}$
- All the Bayesian analysis is similar to the standard linear model:

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- Now we need to invert $\widetilde{\mathbf{K}}$ of ? dimensions

```
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- We do not need to compute the feature vectors explicitly


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- The Function values corresponding to any number of inputs have a joint Gaussian distribution.


## Sample Functions from the Linear Model

(1) Define $\phi_{i}(x)=\exp \left(-\frac{1}{2}\left(x-\mu_{i}\right)^{2}\right)$, for $\mathfrak{i}=1,2,3$
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## (1) The Gaussian Distribution

2. Bayesian Linear Regression
(3) Gaussian Processes for Regression
(4) Gaussian Processes for Classification
(5) Approximations for Large Datasets
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## Function-space View

## Gaussian Process (GP)

$\mathrm{f}(\mathrm{x})$ is a Gaussian process if for any finite subset of points $\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{N}}$, the function values $f\left(x_{1}\right), \ldots, f\left(x_{N}\right)$ follow a Gaussian distribution.

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- Isotropic: $\varphi\left(\left\|\mathbf{x}-\mathbf{x}^{\prime}\right\|\right)$


## The Squared Exponential (SE) Covariance Function

$$
\kappa\left(\mathbf{x}, \mathrm{x}^{\prime}\right)=\sigma_{s}^{2} \exp \left(-\frac{1}{2}\left(\mathbf{x}-\mathbf{x}^{\prime}\right)^{\top} \mathbf{C}\left(\mathbf{x}-\mathrm{x}^{\prime}\right)\right)
$$

- $\sigma_{s}^{2}$ is the signal variance


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$$
\kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\sigma_{s}^{2} \exp \left(-\frac{1}{2}\left(\mathbf{x}-\mathbf{x}^{\prime}\right)^{\top} \mathbf{C}\left(\mathbf{x}-\mathbf{x}^{\prime}\right)\right)
$$

- $\sigma_{s}^{2}$ is the signal variance
- $\mathbf{C}$ is a symmetric matrix that can have different parameterizations


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- $\mathbf{C}=\operatorname{diag}(\ell)^{-2}$ with $\ell=\left(\ell_{1}, \ldots, \ell_{\mathrm{D}}\right)$ : Automatic Relevance Determination (ARD)
- Each $\ell_{j}$ is known as the characteristic length-scale: distance for which the function values are expected to vary significantly


## The Squared Exponential (SE) Covariance Function

Example


## The Squared Exponential (SE) Covariance Function

## Example


$\ell=1, \sigma_{s}^{2}=1$
$\ell=0.1, \sigma_{s}^{2}=1$

## The Squared Exponential (SE) Covariance Function

Example

$\ell=1, \sigma_{s}^{2}=1$


$$
\ell=1, \sigma_{s}^{2}=4
$$


$\ell=0.1, \sigma_{\mathrm{s}}^{2}=1$

## The Squared Exponential (SE) Covariance Function

Example



$$
\ell=1, \sigma_{s}^{2}=1
$$

$$
\ell=0.1, \sigma_{s}^{2}=1
$$




$$
\ell=1, \sigma_{s}^{2}=4
$$

$$
\ell=0.1, \sigma_{s}^{2}=4
$$

## Standard GP Regression Model: Predictions (1)

$$
\begin{aligned}
& \text { Data }: \mathcal{D}=\left\{\left(\mathbf{x}_{i}, y_{i}\right)\right\}_{i=1}^{N}, \\
& \text { Input }:\left(\mathbf{x} \in \mathbb{R}_{\mathrm{D} \times \mathrm{D}}, \mathbf{y} \in \mathbb{R}\right. \\
& \text { Goal }: \text { Margets: }(\mathbf{y})_{\mathrm{N} \times 1} \\
& \text {, predictions } \mathbf{f}_{*}=\mathbf{f}\left(\mathbf{x}_{*}\right) \text { at } \mathbf{x}_{*}
\end{aligned}
$$

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\text { Input }: & (\mathbf{X})_{\mathrm{D} \times \mathrm{N}}, \text { Targets: }(\mathbf{y})_{\mathrm{N} \times 1} \\
\text { Goal : } & \text { Make predictions } f_{*}=\mathrm{f}\left(\mathbf{x}_{*}\right) \text { at } \mathbf{x}_{*} \\
& \text { Prior } \mathrm{f}(\mathbf{x}) \sim \operatorname{GP}\left(\mathbf{0}, \kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)\right)
\end{aligned}
$$

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$$

Input: $(\mathbf{X})_{\mathrm{D} \times \mathrm{N}}$, Targets: $(\mathbf{y})_{\mathrm{N} \times 1}$
Goal: Make predictions $f_{*}=f\left(\mathbf{x}_{*}\right)$ at $\mathbf{x}_{*}$
Prior $f(\mathbf{x}) \sim \mathcal{G P}\left(\mathbf{0}, \kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)\right)$
Noise $\quad y=f(x)+\eta \quad \eta \sim \mathcal{N}\left(0, \sigma_{n}^{2}\right)$

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& \text { Noise } \quad \mathrm{y}=\mathrm{f}(\mathbf{x})+\eta \quad \eta \sim \mathcal{N}\left(0, \sigma_{n}^{2}\right)
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- The joint distribution of $y$ and $f_{*}$ is a Gaussian


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- The joint distribution of $y$ and $f_{*}$ is a Gaussian
- We simply need to figure out the covariance structure:

$$
\operatorname{Cov}\left(y_{p}, y_{\mathfrak{q}}\right)=\kappa\left(x_{p}, x_{q}\right)+\sigma_{n}^{2} \delta_{\mathfrak{p q}} \rightarrow \operatorname{Cov}(\mathbf{y})=\mathbf{K}(\mathbf{X}, \mathbf{X})+\sigma_{n}^{2} \mathbf{I}
$$

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& \text { Input }:(\mathbf{X})_{\mathrm{D} \times \mathrm{N}}, \text { Targets: }(\mathbf{y})_{\mathrm{N} \times 1}
\end{aligned}
$$

Goal : Make predictions $f_{*}=f\left(\mathbf{x}_{*}\right)$ at $\mathbf{x}_{*}$ Prior $f(\mathbf{x}) \sim \mathcal{G P}\left(\mathbf{0}, \kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)\right)$ Noise $y=f(x)+\eta \quad \eta \sim \mathcal{N}\left(0, \sigma_{n}^{2}\right)$

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- To get the posterior on $f_{*}$ we need to constrain this distribution to agree with the observed data ( $\mathbf{X}, \mathbf{y}$ )


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Goal : Make predictions $f_{*}=f\left(\mathbf{x}_{*}\right)$ at $\mathbf{x}_{*}$

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$$

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- To get the posterior on $f_{*}$ we need to constrain this distribution to agree with the observed data ( $\mathbf{X}, \mathbf{y}$ )
- This is achieved simply by conditioning: $\mathfrak{p}\left(\mathbf{f}_{*} \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_{*}\right)$


## Standard GP Regression Model: Predictions (2)

$$
\left[\begin{array}{c}
\mathbf{y} \\
\mathbf{f}_{*}
\end{array}\right] \sim \mathcal{N}\left(\begin{array}{cc}
\mathbf{0}, & \mathbf{K}(\mathbf{X}, \mathbf{X})+\sigma_{n}^{2} \mathbf{I} \\
\mathbf{k}\left(\mathbf{X}, \mathbf{x}_{*}\right) \\
\mathbf{k}\left(\mathbf{x}_{*}, \mathbf{X}\right) & \mathrm{k}\left(\mathbf{x}_{*} \mathbf{x}_{*}\right)
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\end{array}\right)
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Denoting $\mathbf{k}_{*}=\mathbf{K}\left(\mathbf{X}, \mathbf{x}_{*}\right)$ and $\widetilde{\mathbf{K}}=\mathbf{K}(\mathbf{X}, \mathbf{X})+\sigma_{\mathrm{n}}^{2} \mathbf{I}$

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\mathbf{k}\left(\mathbf{x}_{*}, \mathbf{X}\right) & \mathrm{k}\left(\mathbf{x}_{*} \mathbf{x}_{*}\right)
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Denoting $\mathbf{k}_{*}=\mathbf{K}\left(\mathbf{X}, \mathbf{x}_{*}\right)$ and $\widetilde{\mathbf{K}}=\mathbf{K}(\mathbf{X}, \mathbf{X})+\sigma_{\mathrm{n}}^{2} \mathbf{I}$ then:

$$
\begin{aligned}
\mathbf{f}_{*} \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_{*} & \sim \mathcal{N}\left(\mathbb{E}\left[\mathbf{f}_{*}\right], \mathbb{V}\left[\mathbf{f}_{*}\right]\right), \\
\mathbb{E}\left[\mathbf{f}_{*}\right] & =\mathbf{k}_{*}^{\top} \widetilde{\mathbf{K}}^{-1} \mathbf{y} \\
\mathbb{V}\left[\mathbf{f}_{*}\right] & =\mathrm{K}\left(\mathbf{x}_{*}, \mathbf{x}_{*}\right)-\mathbf{k}_{*}^{\top} \widetilde{\mathbf{K}}^{-1} \mathbf{k}_{*} .
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- Say $\boldsymbol{\alpha}=\left(\mathbf{K}+\sigma_{n}^{2} \mathbf{I}\right)^{-1} \mathbf{y}$ then: $\mathbb{E}\left[f_{*}\right]=\sum_{i=1}^{N} \alpha_{i} \kappa\left(\mathbf{x}_{i}, \mathbf{x}_{*}\right)$ is a linear combination of N kernel functions: Representer theorem


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- We encountered this predictive distribution before $\qquad$
- $\mathbb{V}\left[f_{*}\right]$ does not depend on $\mathbf{y}$


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- We encountered this predictive distribution before $\qquad$
- $\mathbb{V}\left[f_{*}\right]$ does not depend on $\mathbf{y}$
- In fact we have a Gaussian posterior process


## The Graphical Model for GPs

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Figure from Carl Rasmussen's slides

## The Graphical Model for GPs



Figure from Carl Rasmussen's slides

- Observations $y$ depend on their corresponding latent function $f$


## The Graphical Model for GPs



Figure from Carl Rasmussen's slides

- Observations $y$ depend on their corresponding latent function $f$
- The marginalization property implies that adding a new $\mathbf{x}_{i}^{*}, f_{i}^{*}, y_{i}^{*}$ does not affect the distribution


## Model Selection

- It includes the discrete choice of the functional form for the covariance function and the values for the hyper-parameters.


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- However, we will refer to the set of hyper-parameters $\theta$ as the parameters of the covariance and the noise variance $\sigma_{n}^{2}$
- We can do cross-validation (potential problems?)
- We focus here on the so-called type II maximum likelihood, i.e. we want to maximize the marginal likelihood.
- Integrate out the "parameters" of the GP: (which parameters?)

$$
\begin{aligned}
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- Computational Requirements?


## Automatic Relevance Determination (ARD)

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Learned lengh-scale for irrelevant dimension: $1.0557 \times 10^{5}$

## Other Covariance Functions: Matérn Covariance

$$
\kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2 v}\left\|\mathbf{x}-\mathbf{x}^{\prime}\right\|}{\ell}\right)^{v} \mathcal{K}_{v}\left(\frac{\sqrt{2 v}\left\|\mathbf{x}-\mathrm{x}^{\prime}\right\|}{\ell}\right)
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- Stationary, Isotropic
- $v=1 / 2$ : $\kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\exp \left(-\frac{\left|\mathbf{x}-\mathbf{x}^{\prime}\right|}{\ell}\right)$
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- $v \rightarrow \infty$ : SE covariance


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with $\alpha \rightarrow \infty$ is the SE covariance with length-scale $\ell$.

## Other Covariance Functions: Neural Network Covariance

- Consider a neural network with one hidden layer and $\mathrm{N}_{\mathrm{H}}$ hidden units.
- Under certain assumptions the corresponding stochastic process will converge to a Gaussian Process as $\mathrm{N}_{\mathrm{H}} \rightarrow \infty$.
- For a specific settings of the transfer function of the neural net:

$$
\kappa\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\frac{2}{\pi} \sin ^{-1}\left(\frac{2 \tilde{\mathbf{x}}^{\top} \boldsymbol{\Sigma} \tilde{\mathbf{x}}^{\prime}}{\sqrt{\left(1+2 \tilde{\mathbf{x}}^{\top} \Sigma \tilde{\mathbf{x}}\right)\left(1+2 \tilde{\mathbf{x}}^{\prime \top} \boldsymbol{\Sigma} \tilde{\mathbf{x}}^{\prime}\right)}}\right)
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## Other Covariance Functions: Periodic, Smooth Functions

We can create a distribution over periodic functions of $x$ by using the mapping $\mathbf{u}(x)=(\cos (x), \sin (x))$ and then use the SE covariance on $\mathbf{u}$ space. This gives rise to:

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This is called warping and can also be used to introduce non-stationarity.
(1) The Gaussian Distribution
(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression
(4) Gaussian Processes for Classification
(5) Approximations for Large Datasets
(6) Current Research
(7) Conclusions

## Gaussian Process Classification: Introduction

- Targets are discrete


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- Generative v discriminative + and - ?


## Linear Models for Classification

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\begin{aligned}
& \text { Data : } \mathcal{D}=\left\{\left(\mathbf{x}_{i}, y_{i}\right)\right\}_{i=1}^{N}, \mathbf{x} \in \mathbb{R}^{\mathrm{D}}, \mathrm{y} \in\{-1,+1\} \\
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Goal : Make predictions at $\mathbf{x}_{*}$
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Multi-class case is addressed with a softmax function.

## Gaussian Process Classification (GPC)

(1) Place prior over the latent functions $f(x)$


Sample from a GP

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


Sample from a GP


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

(1) Compute predictive distribution of latent functions:

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p\left(f_{*} \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_{*}\right)=\int p\left(f_{*} \mid \mathbf{X}, \mathbf{x}_{*}, \mathbf{f}\right) p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) \mathrm{d} \mathbf{f}
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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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Figures by Christopher M. Bishop (MLPR, 2006)
Left : $p(z) \propto \exp \left(-z^{2} / 2\right) \sigma(20 z+4)$ and corresponding Gaussian approximation.
Right : Negative logarithms of the corresponding curves.

## The Laplace Approximation to the GP Binary Classifier

Gaussian approximation

$$
p(\mathbf{f} \mid \mathcal{D}, \theta) \approx \mathcal{N}\left(\mathbf{f} \mid \hat{\mathbf{f}}, A^{-1}\right)
$$

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

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Using Newton's method we obtain the following update:

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& \quad \mathbf{f}^{\mathrm{new}}=\left(\mathbf{W}+\mathbf{K}^{-1}\right)^{-1}\left(\frac{\partial \log p(\mathbf{y} \mid \mathbf{f})}{\partial \mathbf{f}}+\mathbf{W} \mathbf{f}\right) \\
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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:

$$
\mathfrak{p}(\mathbf{f} \mid \mathcal{D}, \boldsymbol{\theta}) \approx \mathcal{N}\left(\mathbf{f} \mid \hat{\mathbf{f}},\left(\mathbf{W}+\mathbf{K}^{-1}\right)^{-1}\right)
$$

When is this approximation a good/bad idea?

## Posterior and Predictive Distributions

Recalling the posterior distribution:

$$
\mathfrak{p}\left(\mathrm{f}_{*} \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_{*}\right)=\int p\left(\mathbf{f}_{*} \mid \mathbf{X}, \mathbf{x}_{*}, \mathbf{f}\right) p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) \mathrm{d} \mathbf{f}
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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:

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

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


Do we spend too much effort in modeling $f$ ?
(1) The Gaussian Distribution
(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression

4 Gaussian Processes for Classification
(5) Approximations for Large Datasets
(6) Current Research
(7) Conclusions

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$$

$\mathrm{q}(\mathbf{f} \mid \mathbf{u})$ is the training conditional and $\mathrm{q}\left(\mathbf{f}_{*} \mid \mathbf{u}\right)$ is the test conditional.
Most approximation methods can be defined by:

- Different specifications of these conditionals.
- Different $\mathbf{X}_{\mathbf{u}}$ : 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:

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Hence the predictive distribution is given by:

$$
\mathbf{q}_{\mathrm{SR}}\left(\mathbf{f}_{*} \mid \mathbf{y}\right)=\mathcal{N}\left(\mathbf{K}_{*, \mathbf{u}} \boldsymbol{\Sigma}^{-1} \mathbf{K}_{\mathbf{u}, \mathbf{f}} \mathbf{y}, \mathbf{K}_{*, \mathbf{u}} \boldsymbol{\Sigma}^{-1} \mathbf{K}_{\mathbf{u}, *}\right)
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where $\boldsymbol{\Sigma}=\mathbf{K}_{\mathbf{u}, \mathbf{f}} \mathbf{K}_{\mathbf{f}, \mathbf{u}}+\sigma_{\mathbf{n}}^{2} \mathbf{K}_{\mathbf{u}, \mathbf{u}}$.

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

We can truncate the number of regressors needed:

$$
\mathrm{f}_{\mathrm{SR}}\left(\mathbf{x}_{*}\right)=\mathbf{k}_{*}^{\top} \boldsymbol{\alpha}_{\mathbf{u}} \text { with } \boldsymbol{\alpha}_{\mathbf{u}} \sim \mathcal{N}\left(\mathbf{0}, \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}\right)
$$

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

$$
\mathbf{q}_{\mathrm{SR}}(\mathbf{f} \mid \mathbf{u})=\mathcal{N}\left(\mathbf{K}_{\mathbf{f}, \mathbf{u}} \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{u}, \mathbf{0}\right) \quad \mathrm{q}_{\mathrm{SR}}\left(\mathbf{f}_{*} \mid \mathbf{u}\right)=\mathcal{N}\left(\mathbf{K}_{*, \mathbf{u}} \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{u}, \mathbf{0}\right)
$$

Hence the predictive distribution is given by:

$$
\mathbf{q}_{\mathrm{SR}}\left(\mathbf{f}_{*} \mid \mathbf{y}\right)=\mathcal{N}\left(\mathbf{K}_{*, \mathbf{u}} \boldsymbol{\Sigma}^{-1} \mathbf{K}_{\mathbf{u}, \mathbf{f}} \mathbf{y}, \mathbf{K}_{*, \mathbf{u}} \boldsymbol{\Sigma}^{-1} \mathbf{K}_{\mathbf{u}, *}\right)
$$

where $\boldsymbol{\Sigma}=\mathbf{K}_{\mathbf{u}, \mathbf{f}} \mathbf{K}_{\mathbf{f}, \mathbf{u}}+\sigma_{\mathbf{n}}^{2} \mathbf{K}_{\mathbf{u}, \mathbf{u}}$.

- 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:

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


## Projected Processes (PP)

$$
\mathrm{q}_{\mathrm{PP}}(\mathbf{f} \mid \mathbf{u})=\mathcal{N}\left(\mathbf{K}_{\mathbf{f}, \mathbf{u}} \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{u}, \mathbf{0}\right) \quad \mathrm{q}_{\mathrm{PP}}\left(\mathbf{f}_{*} \mid \mathbf{u}\right)=\mathfrak{p}\left(\mathbf{f}_{*} \mid \mathbf{u}\right)
$$

- Inducing variables are a subset of training points
- As in SR, it imposes a deterministic training conditional but (unlike $S R$ ) 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
PITC : Partially 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


## (1) The Gaussian Distribution

2. Bayesian Linear Regression
(3) Gaussian Processes for Regression
(a) Gaussian Processes for Classification
(5) Approximations for Large Datasets
(6) Current Research

## 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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- Very little data on test task
- 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 $m$ axis) are correlated (cf independent draws over sample functions)

## Inter-task Tying by Hyper-parameter Sharing



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


## Multi-task GP

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

$$
\begin{aligned}
& \left\langle f_{\ell}(x) f_{m}\left(x^{\prime}\right)\right\rangle=K_{\ell m}^{f} k^{\mathrm{x}}\left(x, x^{\prime}\right) \quad y_{i \ell} \sim \mathcal{N}\left(f_{\ell}\left(x_{i}\right), \sigma_{\ell}^{2}\right), \\
& K^{f}: \text { PSD matrix that specifies the inter-task similarities } \\
& \mathrm{k}^{x}: \text { Covariance function over inputs } \\
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Correlations between tasks modelled directly via $\mathrm{K}^{\mathrm{f}}$

## Multi-task GP Models

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- Block diagonal: Implements task clustering. Cluster structure can be specified a priori. e.g. $\mathrm{K}^{f}$ is diagonal (all tasks are independent)
- Mixture: All functions are independent except for one, which is a mixed version of the others. Effective for transferring to a new task:

$$
\mathrm{K}^{\mathrm{f}}=\left(\begin{array}{cc}
\mathrm{I} & \boldsymbol{\pi} \\
\boldsymbol{\pi}^{\top} & \boldsymbol{\pi}^{\top} \boldsymbol{\pi}
\end{array}\right)
$$

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

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



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- Need to be controlled while having different loads (tasks)


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\tau_{\mathfrak{j}}^{\mathrm{m}}(\mathbf{x})=\mathbf{z}_{\mathfrak{j}}(\mathbf{x})^{\top} \rho_{j}^{m}
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$$

$\Downarrow$
MTGP prior $\left\langle\tau_{j}^{m}(\mathbf{x}) \tau_{\mathfrak{j}}^{\mathfrak{m}^{\prime}}\left(\mathbf{x}^{\prime}\right)\right\rangle=\left(\mathrm{K}_{\mathrm{j}}^{\rho}\right)_{\mathfrak{m} \mathfrak{m}^{\prime}} \mathrm{k}_{\mathfrak{j}}^{\mathrm{x}}\left(\mathrm{x}, \mathrm{x}^{\prime}\right)$

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The MTGP model matches the correlations between torque functions

## Other Non-Gaussian Likelihood Models

- We have encountered this in GP classification
- Ordinal regression: Chu and Ghahramani, JMLR 2005
- Preference Learning: Chu and Ghahramani, ICML 2005
- Preference Elicitation (PE): Bonilla et al, NIPS 2010 (to appear)
- Make optimal recommendations to users by actively querying their preferences.
- Bayesian decision-theoretic PE approach
- Correlated GP prior over user's latent utility functions
- Reduce elicitation burden by leveraging information from previous users


## Latent Variable Models

The Gaussian Process Latent Variable Model (GPLVM; Lawrence, NIPS 2004) is a probabilistic model for non-linear dimensionality reduction.

- Main idea: Some high-dimensional data can be embedded into a low-dimensional non-linear manifold.
- model each dimension of $\left\{\mathbf{x}_{i}\right\}_{i=1}^{N}$ with a corresponding latent point $\mathbf{z}_{i}$ through a non-linear mapping.
- Use an independent GP for this mapping
- Likelihood maximization in order to find the latent projection $\mathbf{z}_{\mathrm{i}}$
- GP models for pose estimation: http://grail.cs.washington.edu/projects/styleik


## Modeling of Human Poses with GPLVM

Grochow et al, SIGGRAPH 2004

- Style-Based Inverse Kinematics: Given a set of constraints, produce the most likely pose.
- Feature vectors are derived from pose information (e.g from mo-cap data).
- joint angles, vertical orientation, velocity and accelerations.
- The problem is inherently underdetermined but some poses are more likely than others.
- Low dimensional representations are learned from previous poses using GPLVM
- 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

## (1) The Gaussian Distribution

(2) Bayesian Linear Regression
(3) Gaussian Processes for Regression

4 Gaussian Processes for Classification
(5) Approximations for Large Datasets
(6) Current Research
(7) Conclusions

## Conclusions and Future Directions

- 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
- More work on design of covariance functions needed
- Towards real large scale GPs
- Dealing with non-standard settings, e.g. preference learning and multi-task learning
- Dealing with structured data


## GP Quiz

