ML for Econometricians
Gaussian Process Classification and Optimization

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Lecture overview

- **Large scale GPs**
- **Gaussian Process Classification**
- **Gaussian Process Optimization**

Large scale GPs

- GPs are **computationally challenging**. Need to invert $n \times n$ matrices such as $\left[K(\mathbf{x},\mathbf{x}) + \sigma^2 I\right]^{-1}$. **Scales as $O(n^3)$**.
- **Banded covariance functions**.
  - Special covariance functions that makes $K(\mathbf{x},\mathbf{x})$ sparse.
  - Observations more than a certain distance apart are uncorrelated.
  - Sparse matrix algebra.
  - Still $O(n^3)$, but faster for a given n.
- **Inducing variables**
  - Introduce m latent **inducing variables** $\mathbf{u} = \{u_1, ..., u_m\}$ with corresponding inducing inputs $\mathbf{X}_u = \{\mathbf{x}_{u_1}, \mathbf{x}_{u_2}, ..., \mathbf{x}_{u_m}\}$. Pseudo inputs.
  - The **Fully Independent Conditional** (**FIC**) method *assumes*

$$p(\mathbf{f}|\mathbf{X}, \mathbf{X}_u, \mathbf{u}, \theta) = \prod_{i=1}^{n} p_i(f_i|\mathbf{X}, \mathbf{X}_u, \mathbf{u}, \theta)$$

  - Computations are now $O(m^2 n)$. If $m \ll n$, much faster computations.
  - **Partially Independent Conditional** (**PIC**).

Classification with logistic regression

- **Classification**: **binary response** $y \in \{-1, 1\}$ predicted by features $\mathbf{x}$.
- Example: linear logistic regression

$$Pr(y = 1|\mathbf{x}) = \lambda(\mathbf{x}^T\mathbf{w})$$

where $\lambda(z)$ is the logistic **link function**

$$\lambda(z) = \frac{1}{1 + \exp(-z)}$$

- $\lambda(z)$ 'squashes' the linear prediction $\mathbf{x}^T\mathbf{w} \in \mathbb{R}$ into $\lambda(\mathbf{x}^T\mathbf{w}) \in [0, 1]$.
- Logistic regression has **linear decision boundaries**.

GP classification

- **GP**: replace $\mathbf{x}^T\mathbf{w}$ by $f(\mathbf{x})$ where

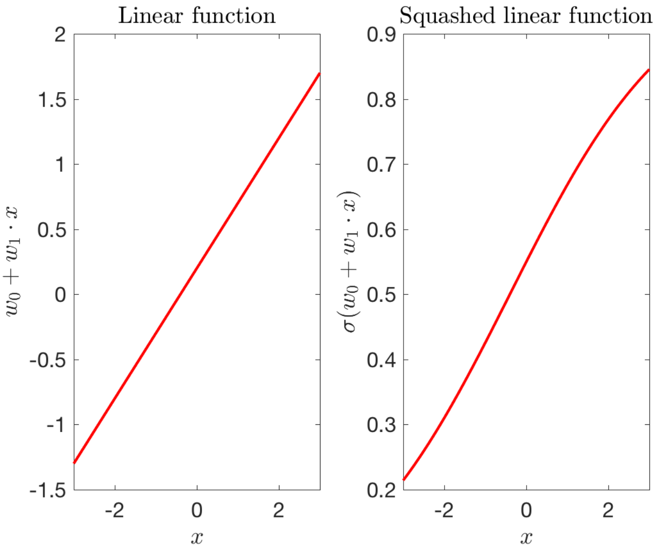
$$f(\mathbf{x}) \sim GP(0, k(\mathbf{x}, \mathbf{x}')).$$

- Squash f through logistic function

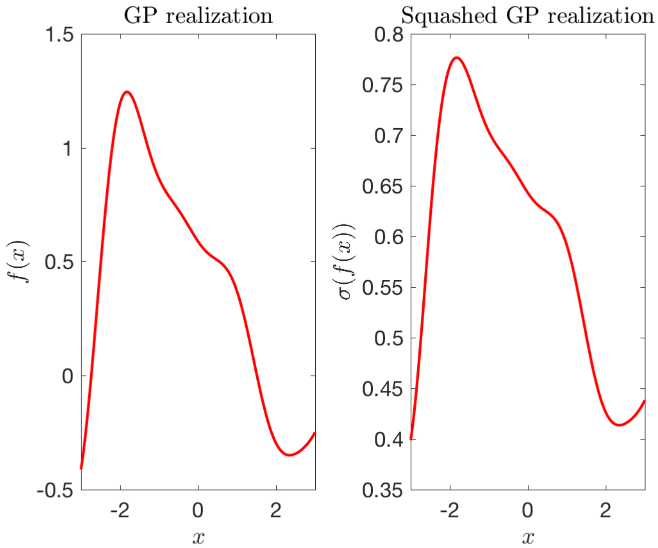
$$Pr(y = 1|\mathbf{x}) = \lambda(f(\mathbf{x}))$$

- Decision boundaries are now non-parametric (GP). Flexible.
- GP Probit: use normal CDF, $\Phi(z)$, as squashing function.

Squashing a linear function



Squashing a GP function



GP classification - inference

- **Prediction** for a test case $\mathbf{x}_*$

$$Pr(y_* = 1|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) = \int \sigma(f_*) p(f_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) df_*$$

  where $\sigma(f_*)$ is some sigmoidal function and f_* is f at $\mathbf{x}_*$.
- The posterior distribution of f_* is

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

  with the posterior of $\mathbf{f}$ from the training data.

$$p(\mathbf{f}|\mathbf{X}, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{X}, \mathbf{f}) p(\mathbf{f}|\mathbf{X}).$$

- Posterior $p(\mathbf{f}|\mathbf{X}, \mathbf{y})$ is no longer analytically tractable. Alternatives:
  - Laplace approximation
  - Expectation propagation
  - MCMC/HMC

Markov Chain Monte Carlo

- Metropolis-Hastings (or Hamiltonian MC) to **sample from training posterior**

$$\mathbf{f}|\mathbf{x}, \mathbf{y}, \theta$$

Produces $\mathbf{f}^{(1)}, ..., \mathbf{f}^{(N)}$ draws.

- For each $\mathbf{f}^{(i)}$, **sample the test posterior** $\mathbf{f}_*$ from

$$\mathbf{f}_*|\mathbf{f}^{(i)}, \mathbf{x}, \mathbf{x}_* \sim N\left(K(\mathbf{x}_*, \mathbf{x})K(\mathbf{x}, \mathbf{x})^{-1}\mathbf{f}^{(i)}, K(\mathbf{x}_*, \mathbf{x}_*) - K(\mathbf{x}_*, \mathbf{x})K(\mathbf{x}, \mathbf{x})^{-1}\right.$$

Note that this does not depend on $\mathbf{y}$ since we condition on $\mathbf{f}$.
Noise-free GP fit. Produces $\mathbf{f}_*^{(1)}, ..., \mathbf{f}_*^{(N)}$ draws.

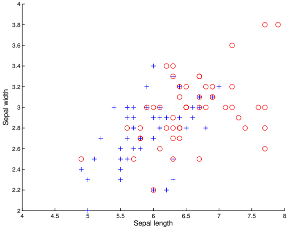
- For each $\mathbf{f}_*^{(i)}$, **sample a prediction** from

$$p(\mathbf{y}_*|\mathbf{f}_*^{(i)}, \theta).$$

Produces a draws from the predictive distribution $p(\mathbf{y}_*|\mathbf{x}_*, \mathbf{x}, \mathbf{y}, \theta)$.

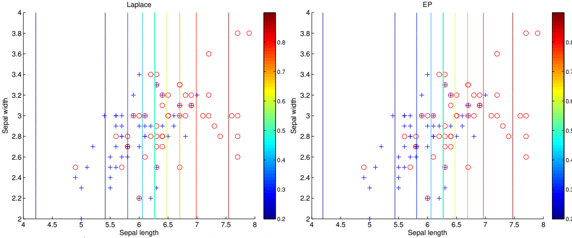
- Straightforward (at least in principle) to also **sample the hyperparameters** θ. Elliptical slice sampling.

IRIS DATA - SEPAL - SE KERNEL WITH ARD

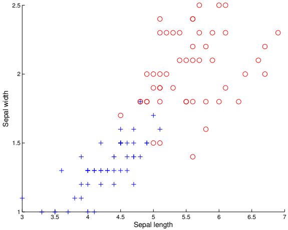


Laplace: $\hat{\ell}_1 = 1.7214, \hat{\ell}_2 = 185.5040, \sigma_f = 1.4361$

EP: $\hat{\ell}_1 = 1.7189, \hat{\ell}_2 = 55.5003, \sigma_f = 1.4343$

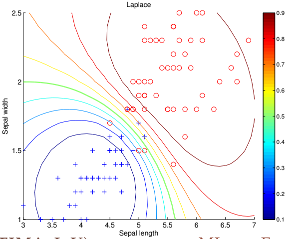


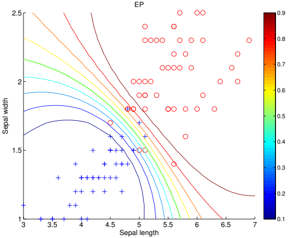
Iris data - petal - SE kernel with ARD



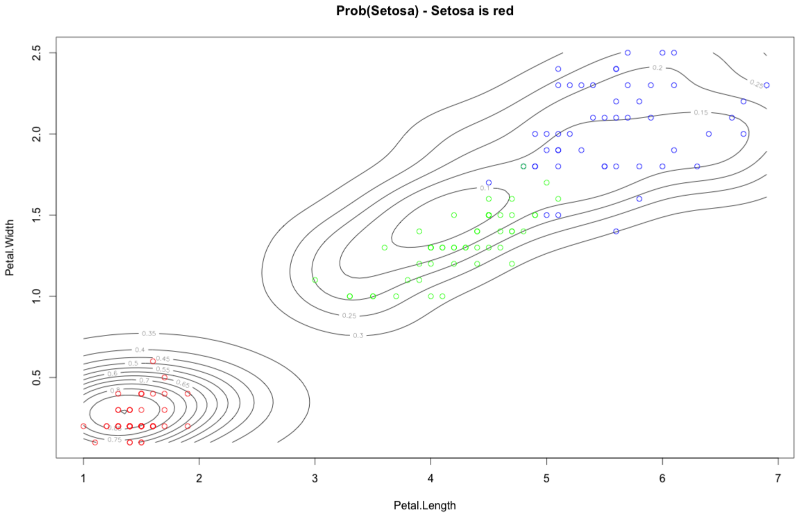
Laplace: $\hat{\ell}_1 = 1.7606, \hat{\ell}_2 = 0.8804, \sigma_f = 4.9129$

EP: $\hat{\ell}_1 = 2.1139, \hat{\ell}_2 = 1.0720, \sigma_f = 5.3369$





IRIS DATA - PETAL - ALL THREE CLASSES



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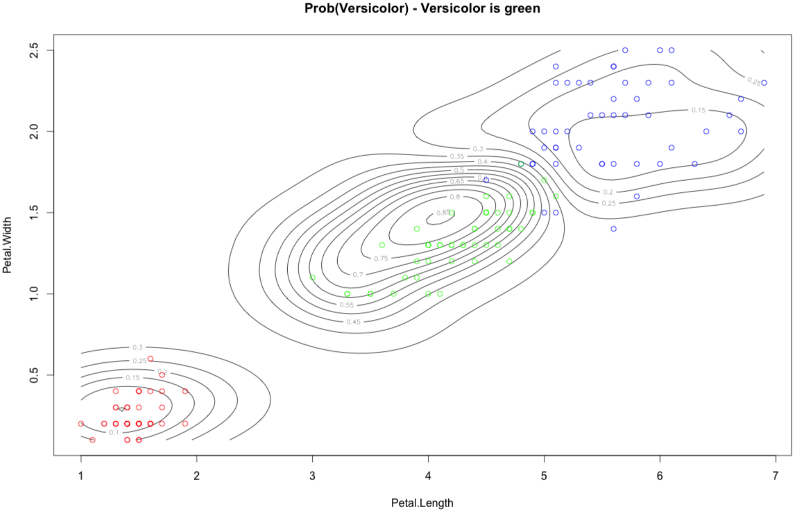

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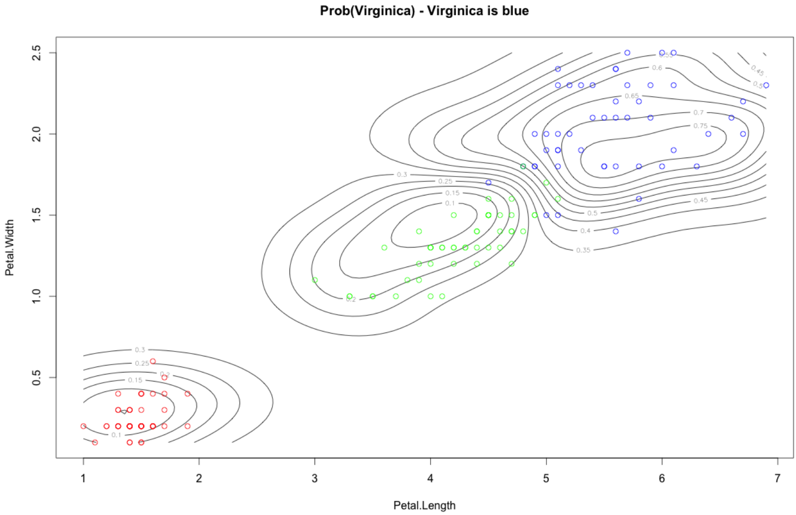
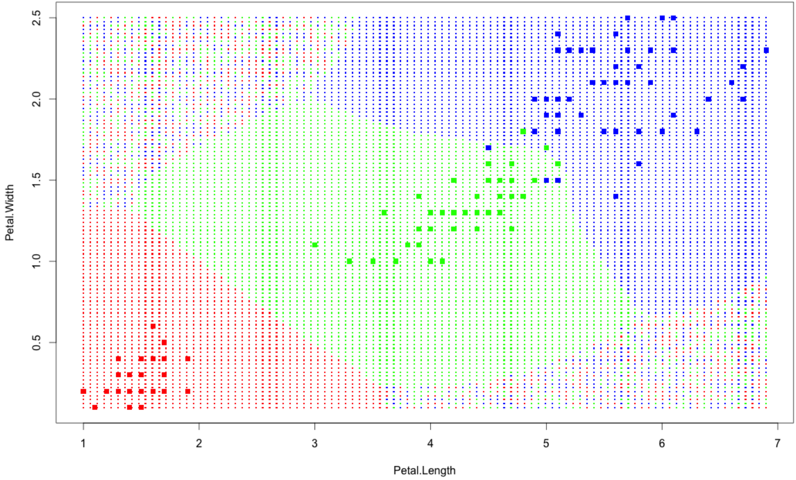
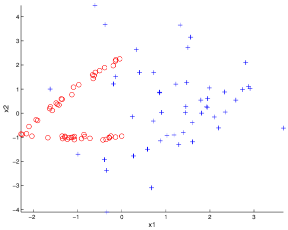


Iris data - petal - decision boundaries

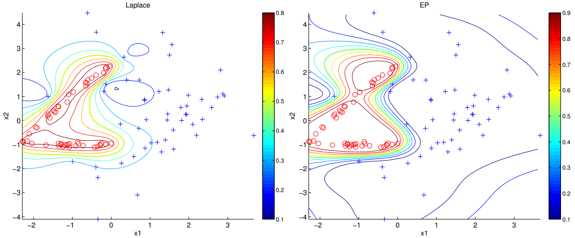


TOY DATA - SE KERNEL WITH ARD



$$\text{Laplace: } \hat{\ell}_1 = 0.7726, \hat{\ell}_2 = 0.6974, \sigma_f = 11.7854$$

$$\text{EP:} \hat{\ell}_1 = 1.2685, \hat{\ell}_2 = 1.0941, \sigma_f = 17.2774$$



Gaussian Process Optimization (GPO)

- **Aim**: minimization of function

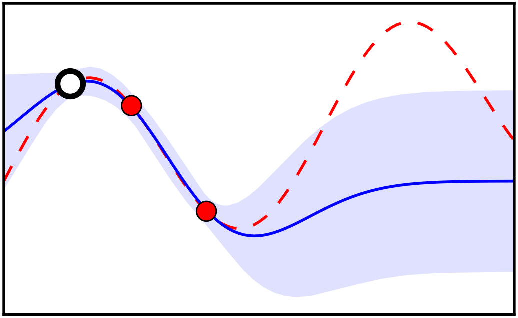
$$\text{argmin}_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$$

- Typical applications: **expensive function evaluation** in < 20 dimensions. **Hyperparameter estimation**.

- **GPO idea**:
  - Assign GP prior to the unknown function f.
  - Evaluate the function at some values $x_1, x_2, ..., x_n$.
  - Update to posterior $f|x_1, ..., x_n \sim GP(\mu, K)$. Noise-free model.
  - Use the GP posterior of f to find a new evaluation point x_{n+1}. **Explore** vs **Exploit**.
  - Iterate until the change in optimum is lower that some tolerance.

- **Bayesian Optimization**. Bayesian Numerics. Probabilistic numerics.

Explore-Exploit Illustration



Acquisition functions

- **Probability of Improvement (PI)**

$$a_{PI}\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right) \equiv \Pr\left(f(\mathbf{x}) < f(\mathbf{x}_{best})\right) = \Phi(\gamma(\mathbf{x}))$$

where

$$\gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{best}) - \mu\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right)}{\sigma\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right)}$$

- **Expected Improvement (EI)**

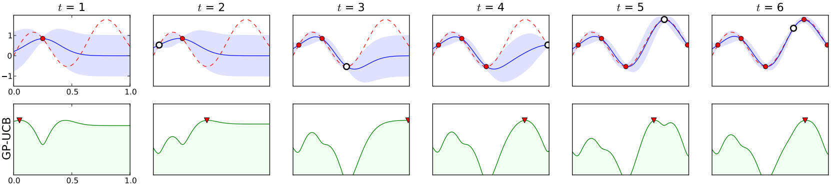
$$a_{EI}\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right) = \sigma\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right)\left[\gamma(\mathbf{x})\Phi(\gamma(\mathbf{x})) + \mathcal{N}\left(\gamma(\mathbf{x});0,1\right)\right]$$

- **Lower Confidence Bound (LCB)**

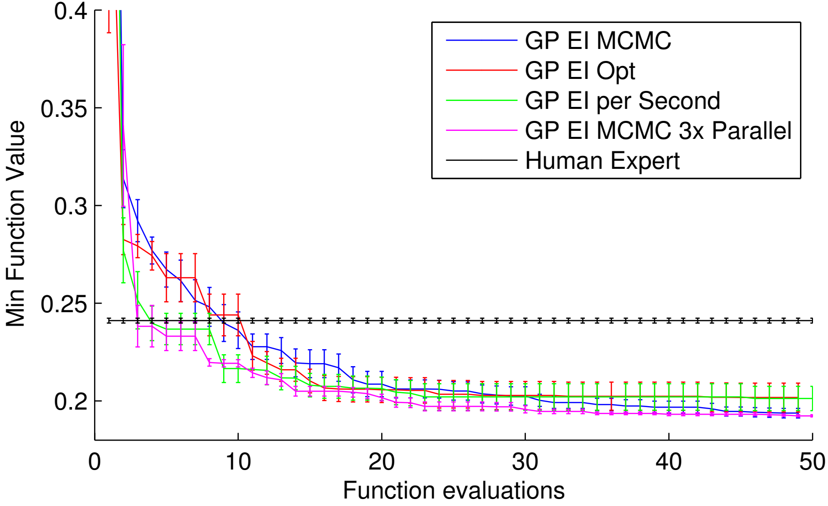
$$a_{EI}\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right) = \mu\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right) - \kappa\cdot\sigma\left(\mathbf{x};\{\mathbf{x}_n,y_n\},\theta\right)$$

- Note: need to maximize the acquisition function to choose $\mathbf{x}_{next}$. Non-convex, but cheaper and simpler than original problem.

Acquisition functions from Brochu et al



ConvNets - Snoek et al (NIPS, 2012)



GPs can be used everywhere

- **Heteroscedastic GP regression**

$$y = f(x) + \exp\left[g(x)\right]\epsilon$$

so where $f \sim GP\left[m_f(x), k_f(x, x')\right]$ independently of $g \sim GP\left[m_g(x), k_g(x, x')\right]$.

- GP for **density estimation**

$$p(x) = \frac{\exp\left[f(x)\right]}{\int_{\mathbb{R}} \exp\left[f(t)\right] dt}$$

where $f \sim GP\left[m(x), k(x, x')\right]$. Appealing mean function: $m(x) = -\frac{1}{2\theta_2}(x - \theta_1)^2$ [i.e. best guess is a normal density].

- **Shared latent GP** for **dependent multivariate data** ($k \ll p$)

$$\begin{pmatrix} y_1(\mathbf{x}) \\ \vdots \\ y_p(\mathbf{x}) \end{pmatrix} = \underset{p \times k}{\mathbf{L}} \begin{pmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_k(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} g_1(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_p \end{pmatrix}$$