Gaussian Processes (Contd)

Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

Jan 30, 2019

Announcement

- Quiz 1 tomorrow - Jan 31, 7pm-8pm
- Y14, Y15, Y18: RM-101
- Y16, Y17: KD-101
- Bring a pencil and eraser (answers to be written on the question paper itself)
- Do not bring anything else

Recap: Bayesian Modeling of Nonlinear Functions

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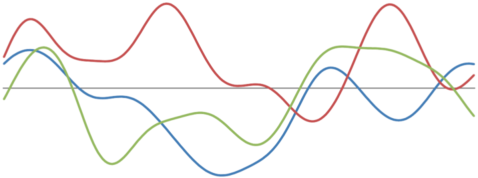
  - Bayesian Neural Networks (infer posterior over NN weights; compute posterior predictive)
  - Gaussian Processes (Bayesian modeling + kernels)

Recap: Gaussian Process

- A Gaussian Process is a distribution over functions
- Denoted as $\mathcal{GP}(\mu, \kappa)$; parametrized by a mean function μ and covariance/kernel function κ



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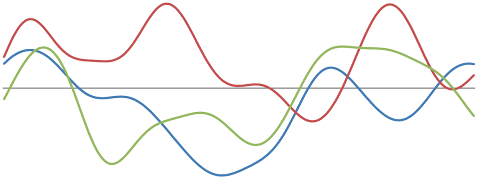

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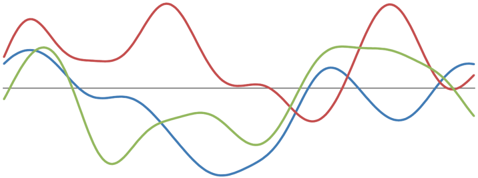

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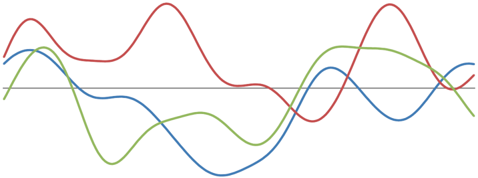

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    - $\kappa(.,.)$ is a function that computes similarity between two inputs

Recap: Gaussian Process

- For $f \sim \mathcal{GP}(\mu, \kappa)$, f's values at any finite set of input $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ are jointly Gaussian

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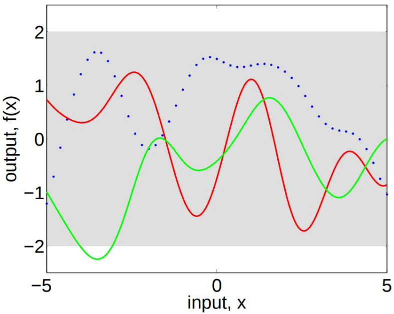
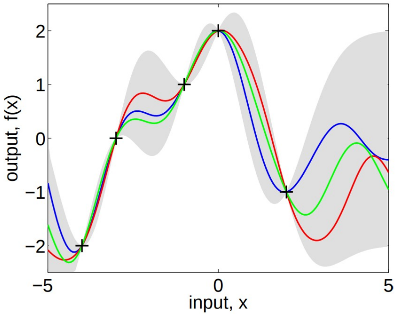
GP: A Visualization



Some functions drawn from a GP prior (note: Blue dots are values of a randomly drawn function at a small number of inputs; the solid curves are generated by evaluating the functions at a large # of inputs)



Some functions drawn from the GP posterior after observing 5 (x,f(x)) pairs

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- Using the same result, the marginal distribution $p(y_*) = \mathcal{N}(y_*|0, \kappa(\boldsymbol{x}_*, \boldsymbol{x}_*) + \sigma^2)$

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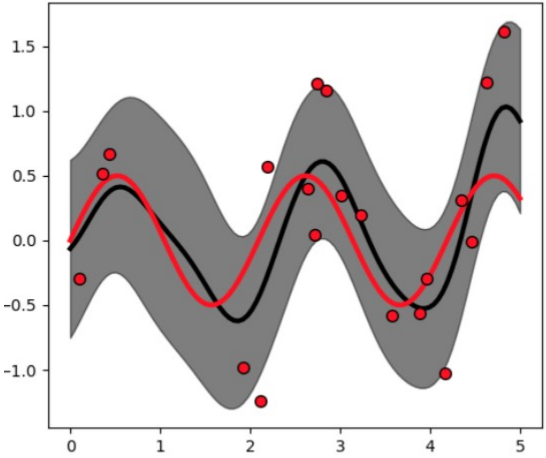
- Can interpret predictive mean μ_* as kernelized SVM or nearest neighbor based prediction

GP Regression: An Illustration



Red curve: True function
Red points: Noisy training examples
Black curve: Predictive mean
Shaded part: Predictive variance

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$$\log p(\mathbf{y}|\sigma^2, \theta) = -\frac{1}{2}\log|\sigma^2\mathbf{I}_N + \mathbf{K}_\theta| - \frac{1}{2}\mathbf{y}^\top(\sigma^2\mathbf{I}_N + \mathbf{K}_\theta)^{-1}\mathbf{y} + \text{const}$$

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- This in general is not as easy to compute as in case of GP regression
  - $p(f_*|\boldsymbol{f})$ is still not a problem (will be Gaussian)
  - $p(\mathbf{f}|\boldsymbol{y}) \propto p(\boldsymbol{f})p(\boldsymbol{y}|\boldsymbol{f})$ will require approximation (e.g., Laplace, MCMC, variational, etc.)
  - The overall integral will require approximation as well

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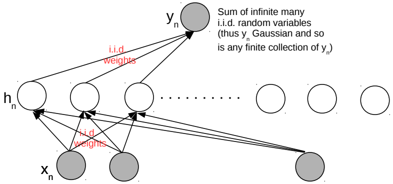
- GPs equivalent to infinitely-wide single hidden-layer neural net (under some technical conditions)

Neural Networks and Gaussian Processes

- An infinitely-wide single hidden layer NN with i.i.d. priors on weights = a Gaussian Process
- Shown formally by (Radford Neal, 1994)[2]. Based on a simple application of central limit theorem



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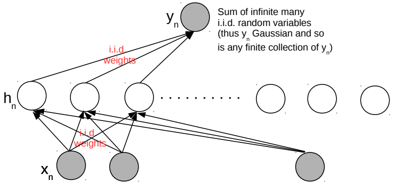

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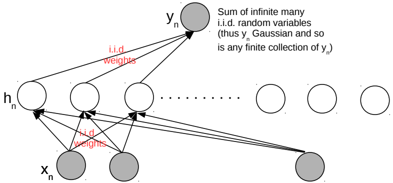

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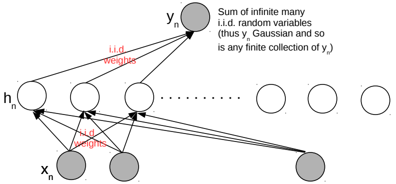

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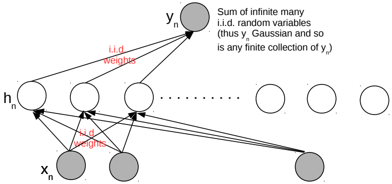

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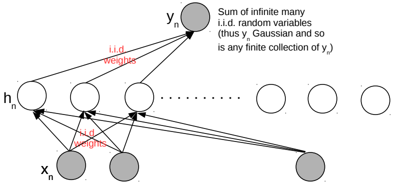

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- Connection recently generalized to infinitely wide multiple hidden layer NN (Lee et al, 2018)[3]

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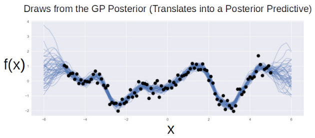

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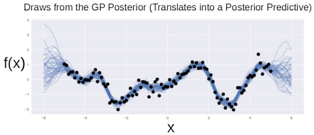

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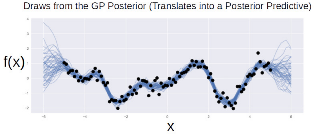

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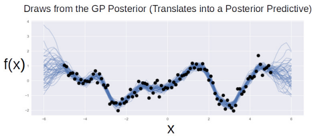

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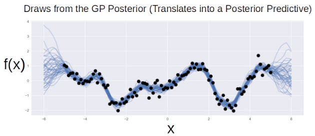

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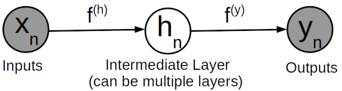
- Many mature implementations of GP exist. You may check out
  - GPML (MATLAB), GPsuff (MATLAB/Octave), GPy (Python), GPyTorch (PyTorch)

Other Recent Advances on Gaussian Processes

- Deep Gaussian Processes (DGP)
  - Akin to a deep neural network where each hidden node is modeled by a GP



  - A nice alternative to linear transform + nonlinearity based neural nets, e.g., $\boldsymbol{h} = \tanh(\mathbf{W}\boldsymbol{x})$

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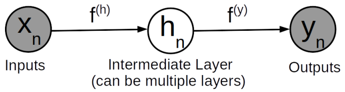

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Other Recent Advances on Gaussian Processes

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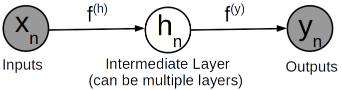

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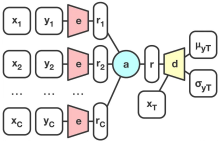
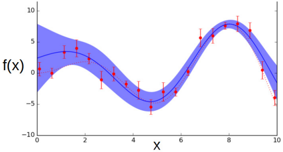
- Neural Processes and Conditional Neural Processes (GP + neural nets): Most recent development



GPs are very versatile!

- GPs enable us to learn nonlinear functions while also capturing the uncertainty



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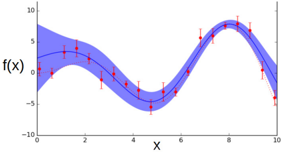

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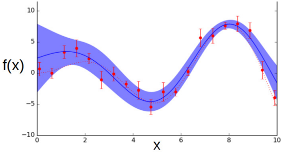

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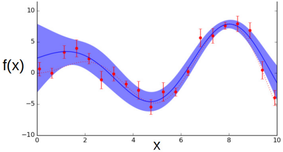

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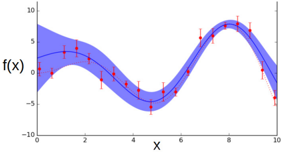

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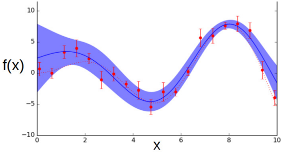

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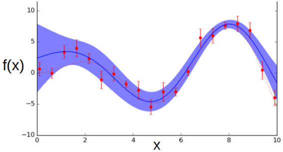

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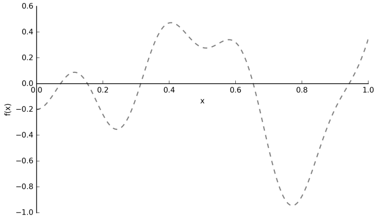

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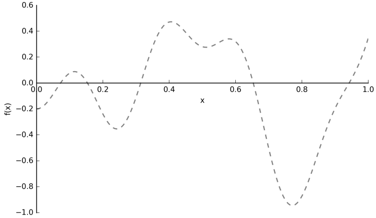

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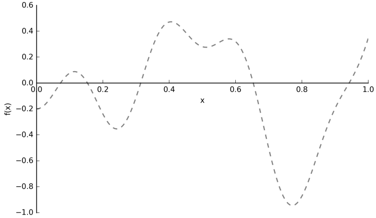

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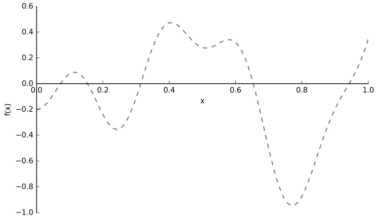

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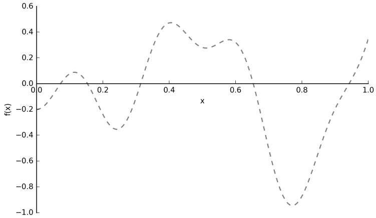

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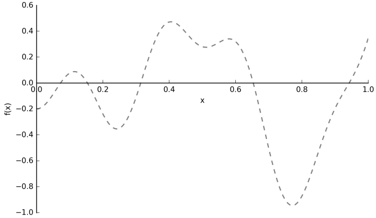

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- Will look at it in more detail later this semester