LECTURE 11: From Interpolation to Regression to Gaussian Process

- So far we were mostly doing linear or nonlinear regression of data points with simple small basis (for example, linear function $y = ax+b$)
- The basis can be arbitrarily large and can be defined in many different ways: we do not care about values of a, b … but about predictions for y
- This is the task of machine learning
- Interpolation can be viewed as regression without noise (but still sparse sampling of data)
- There are many different regressions

Interpolation

- Goal: we have function $y = f(x)$ defined at points $y_i = f(x_i)$, and we want to know its value at any x. For now we will assume solution goes through x_i's
- Why? Perhaps it is very expensive to evaluate it everywhere. Or perhaps we really do not know it.
- Local interpolation: use a few nearby points
- Example: polynomial interpolation $f(x) = \Sigma_{i=1}^{N} a_i x^i$
- How do we choose N? Higher N better for smooth functions and worse for sharp kinks

Differentiability

- Lagrange formula for polynomial interpolation:

$$P(x) = \frac{(x-x_1)(x-x_2)...(x-x_{M-1})}{(x_0-x_1)(x_0-x_2)...(x_0-x_{M-1})} y_0 + \frac{(x-x_0)(x-x_2)...(x-x_{M-1})}{(x_1-x_0)(x_1-x_2)...(x_1-x_{M-1})} y_1 + \cdots + \frac{(x-x_0)(x-x_1)...(x-x_{M-2})}{(x_{M-1}-x_0)(x_{M-1}-x_1)...(x_{M-1}-x_{M-2})} y_{M-1}$$

- Polynomial interpolation does not guarantee that derivatives are differentiable everywhere.
- Stiffer solution are splines, where we enforce derivatives to be continuous
- Most popular is cubic spline where 1st derivatives are smooth and 2nd derivatives are continuous

Cubic Spline

- Start with piecewise linear interpolation

$$y = Ay_j + By_{j+1} \qquad A \equiv \frac{x_{j+1} - x}{x_{j+1} - x_j} \qquad B \equiv 1 - A = \frac{x - x_j}{x_{j+1} - x_j}$$

- This will not have 2nd derivative continuous: it is zero inside intervals and infinite at x_i
- But we can add another interpolation of 2nd derivatives y''. If we also arrange it to be 0 at x_i then we do not spoil linear interpolation above.
- This has a unique solution:

$$y = Ay_j + By_{j+1} + Cy''_j + Dy''_{j+1}$$

$$C \equiv \tfrac{1}{6}(A^3 - A)(x_{j+1} - x_j)^2 \qquad D \equiv \tfrac{1}{6}(B^3 - B)(x_{j+1} - x_j)^2$$

- Note that A and B depend on x

Cubic Spline

- So far we assumed we know y'', but we do not
- We can determine it by requiring continuity of 1st derivatives on both sides of x_i:

$$\frac{dy}{dx} = \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{3A^2 - 1}{6}(x_{j+1} - x_j)y''_j + \frac{3B^2 - 1}{6}(x_{j+1} - x_j)y''_{j+1}$$

$$\frac{x_j - x_{j-1}}{6}y''_{j-1} + \frac{x_{j+1} - x_{j-1}}{3}y''_j + \frac{x_{j+1} - x_j}{6}y''_{j+1} = \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{y_j - y_{j-1}}{x_j - x_{j-1}}$$

- We get N-2 equations for N unknown y_i'', tridiagonal system, *O(N). Each* y_j'' is coupled only to j , j+/-1
- Natural cubic spline: set y_0'' = 0 and y_N'' = 0

Rational Function Expansion

- Spline is mostly used for interpolation
- Polynomials can be used for extrapolation outside the interval (x_0, x_N), but the polynomial with the largest power dominates and results in divergence
- Rational functions can be better for extrapolation: if we know the function goes to 0 we choose $n > m$

$$R_{i(i+1)\ldots(i+m)} = \frac{P_\mu(x)}{Q_\nu(x)} = \frac{p_0 + p_1 x + \cdots + p_\mu x^\mu}{q_0 + q_1 x + \cdots + q_\nu x^\nu}$$

- Rational functions are better for interpolation if the functions has poles (in real or complex plane)
- Rational functions can also be used for analytic work (Pade approximation)

Interpolation on a grid in higher dimension

- Simplest 2d example: bilinear interpolation

$$t \equiv (x_1 - x_{1i})/(x_{1(i+1)} - x_{1i})$$
$$u \equiv (x_2 - x_{2j})/(x_{2(j+1)} - x_{2j})$$

(so that t and u each lie between 0 and 1) and

$$y(x_1, x_2) = (1-t)(1-u)y_0 + t(1-u)y_1 + tuy_2 + (1-t)uy_3$$

- Higher order accuracy: polynomials (biquadratic…)
- Higher order smoothness: bicubic spline

From Spline to B-spline to Gaussian

- We said spline is sparse. We can write basis functions for (cubic) splines (B for basis), so that the solution is a linear combination of them. For cubic B-splines on uniform points

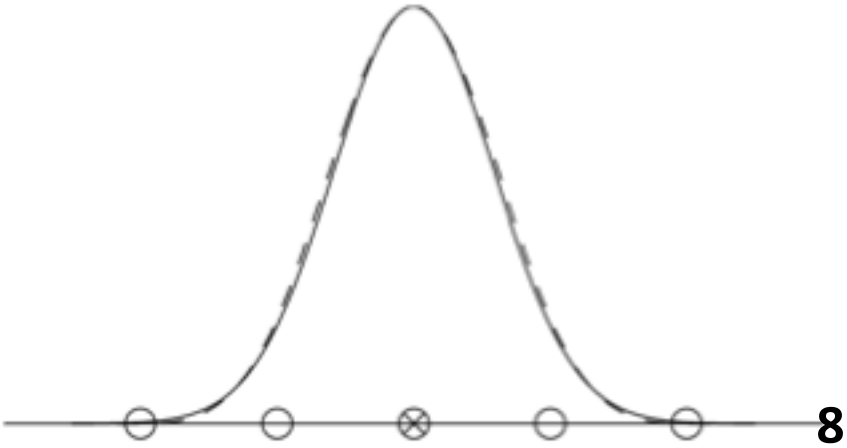
$$\mu(x) = \sum_{h=1}^{H} \beta_h b_h(x)$$

$$b_h(x) = \begin{cases} \frac{1}{6}u^3 & \text{for } x \in (x_h, x_{h+1}), \quad u = (x - x_h)/\delta \\ \frac{1}{6}(1 + 3u + 3u^2 - 3u^3) & \text{for } x \in (x_{h+1}, x_{h+2}), \quad u = (x - x_{h+1})/\delta \\ \frac{1}{6}(4 - 6u^2 + 3u^3) & \text{for } x \in (x_{h+2}, x_{h+3}), \quad u = (x - x_{h+2})/\delta \\ \frac{1}{6}(1 - 3u + 3u^2 - u^3) & \text{for } x \in (x_{h+3}, x_{h+4}), \quad u = (x - x_{h+3})/\delta \\ 0 & \text{otherwise.} \end{cases}$$

- Example: if $x=x_{h+2}$ the weights are 0,1/6,4/6,1/6,0
- Very close to gaussian

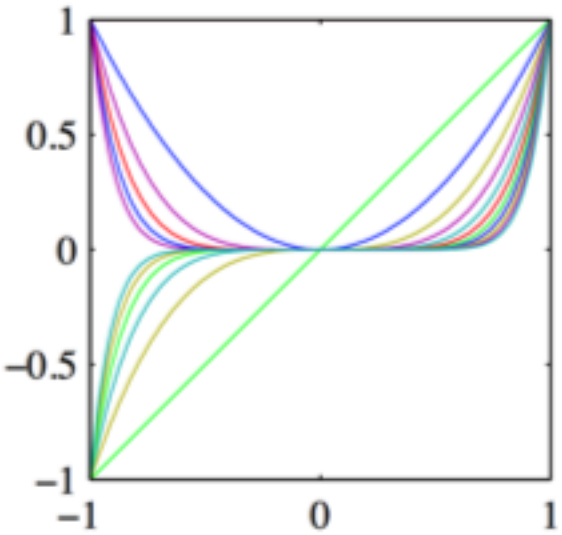
$$b_h(x) = \exp\left(-\frac{|x - x_h|^2}{l^2}\right)$$

- Smoothness vs sparseness:
- Gaussian is infinitely differentiable (i.e. smoother) but not sparse

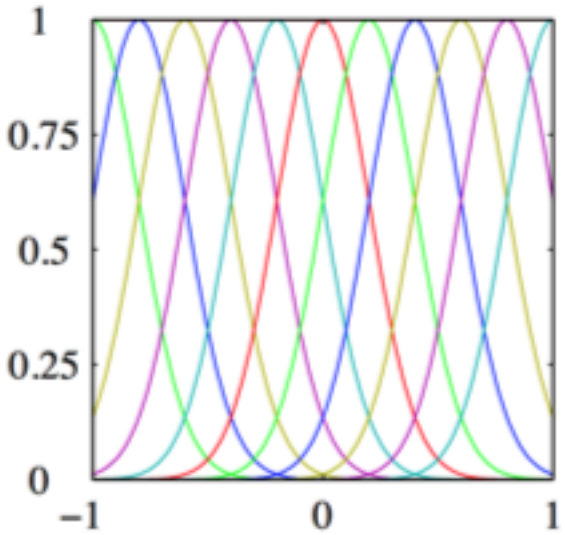


Example of Basis Functions

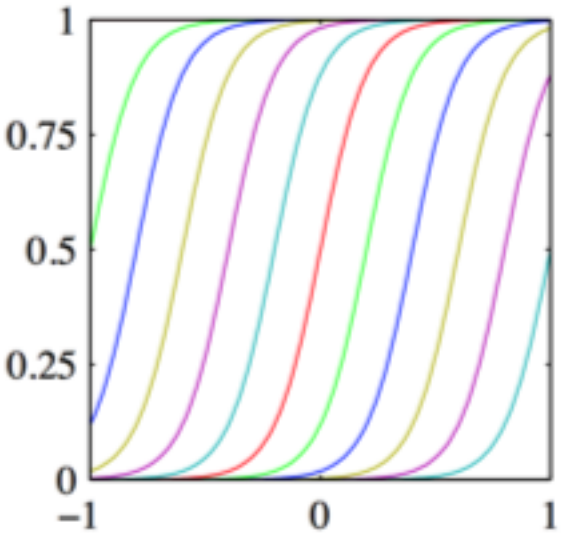
- Polynomial



Spline/Gaussian



Sigmoid



- Sigmoid (used for classification)

$$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right) \text{ with } \sigma(a) = \frac{1}{1+e^{-a}}$$

From Interpolation to Regression

- One can view function interpolation as regression in the limit of zero noise, but still sparse and uniform sampling
- Sparse sampling will induce an error, as will noise
- Both can use the same basis expansion $\phi(x)$
- For regression with noise or sparse sampling we add a regularization term (Tikhonov/ridge/L2, Lasso/L1…), this can prevent overfitting
- $l = \Sigma_{i=1}^{N} [\Sigma_{j=1}^{M} a_j \phi(x_i) - y_i]^2 + \lambda \Sigma_{j=1}^{M} a_j^2$
- The question is how to choose the regularization parameter λ

Bayesian Regression

$$t = \underbrace{y(\boldsymbol{x}, \boldsymbol{w})}_{\text{deterministic}} + \underbrace{\epsilon}_{\text{Gaussian noise}}$$

$$y(x)=\mathbf{w}^{\mathsf{T}}\phi(\boldsymbol{x})$$

- In the Bayesian context we perform regression of coefficients w_j assigning them some prior distribution, such as a gaussian with some precision α. If we also have noise precision β then $\ln p$ is

$$\ln p(\mathbf{w}|\mathbf{t}) = -\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\right)^2 - \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} + \text{const}$$

- So regularizing parameter is $\lambda = \alpha/\beta$

Linear Algebra Solution

- More general prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N) \propto p(\mathbf{t}|\mathbf{w})p(\mathbf{w})$$

- Posterior

$$\left| \begin{array}{rcl} \mathbf{m}_N & = & \mathbf{S}_N(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\Phi^{\mathrm{T}}\mathbf{t}) \\ \mathbf{S}_N^{-1} & = & \mathbf{S}_0^{-1} + \beta\Phi^{\mathrm{T}}\Phi \end{array} \right.$$

- We want to predict at arbitrary t by marginalizing over $\mathbf{w}$

$$p(t|\mathbf{t}, \alpha, \beta) = \int p(t|\mathbf{w}, \beta)p(\mathbf{w}|\mathbf{t}, \alpha, \beta)d\mathbf{w}$$

Prediction for *t*

$$p(t|\mathbf{t},\alpha,\beta) = \int p(t|\mathbf{w},\beta)p(\mathbf{w}|\mathbf{t},\alpha,\beta)d\mathbf{w}$$

$$p(t|\mathbf{w},\beta) = \mathcal{N}(t|y(\mathbf{x},\mathbf{w}),\beta^{-1})$$

$$p(\mathbf{w}|\mathbf{t},\alpha,\beta) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N,\mathbf{S}_N)$$

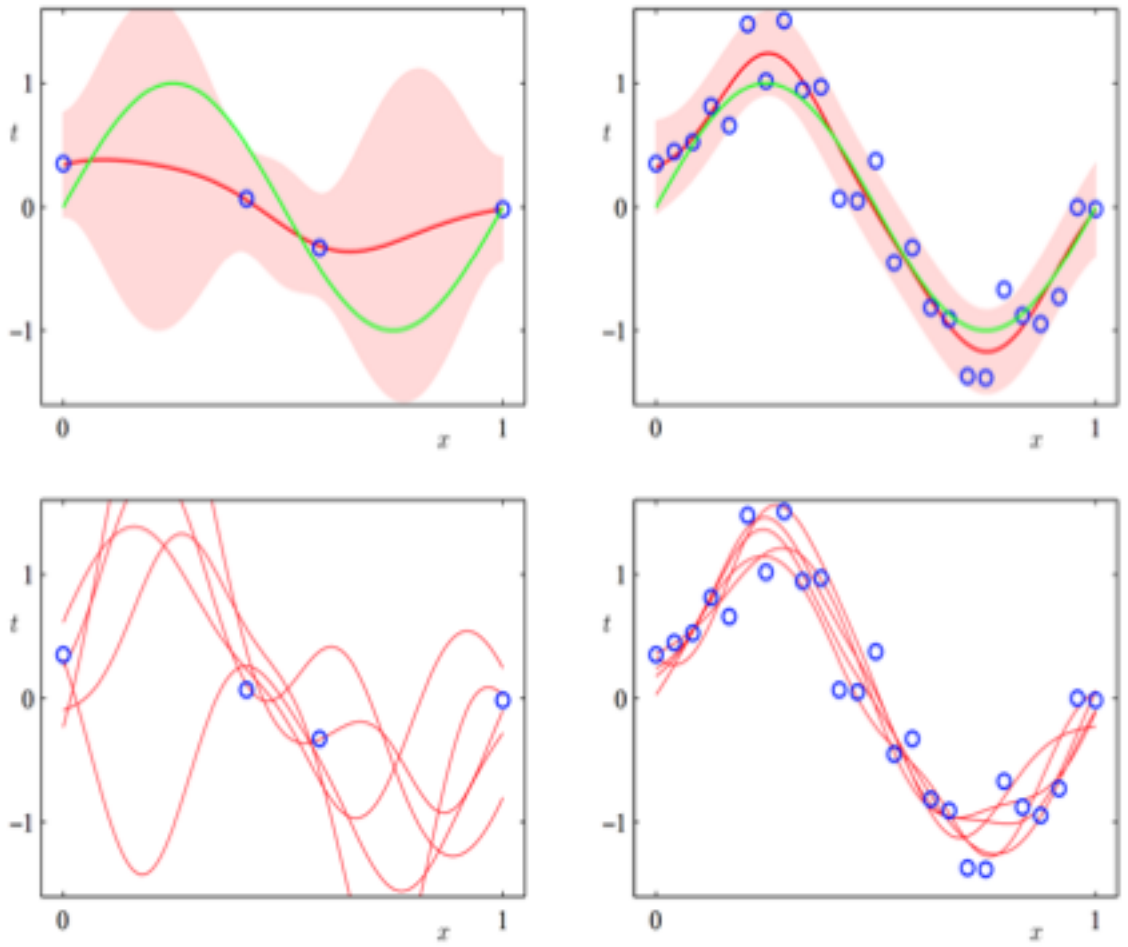
$$p(t|\mathbf{x},\mathbf{t},\alpha,\beta) = \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}}\Phi(\mathbf{x}),\sigma_N^2(\mathbf{x}))$$

$$\sigma_N^2(\mathbf{x}) = \underbrace{\beta^{-1}}_{\text{noise in data}} + \underbrace{\Phi(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\Phi(\mathbf{x})}_{\text{uncertainty in } \mathbf{w}}$$

Examples

no overfit because of regularization

We get error estimate



Kernel Picture

- Kernels work as closeness measure, giving more weight to nearby points. Assuming $m_0 = 0$

$y(\mathbf{x}, \mathbf{m}_N)$ rewrites as $\sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n)\mathbf{t}_n$ where

$$k(\mathbf{x}, \mathbf{x}') = \beta\Phi(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\Phi(\mathbf{x}')$$

Basis functions $\leftrightsquigarrow$ kernel duality

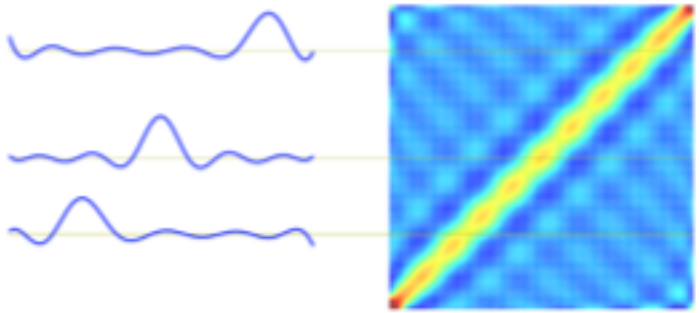
With $\Psi(\mathbf{x}) = \beta^{-1/2}\mathbf{S}_N^{1/2}\Phi(\mathbf{x})$, $k(\mathbf{x}, \mathbf{x}') = \Psi(\mathbf{x})^{\mathrm{T}}\Psi(\mathbf{x}')$

The kernel sums to one (over the training set)

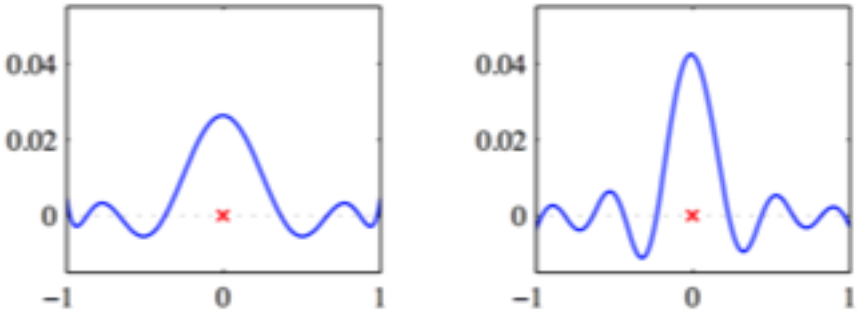
$\mathrm{cov}(y(\mathbf{x}), y(\mathbf{x}')) = \beta^{-1}k(\mathbf{x}, \mathbf{x}')$

Kernel Examples

Kernel from Gaussian basis functions



Kernels at $\mathbf{x} = 0$ for kernels corresponding (left) to the polynomial basis functions and (right) to the sigmoidal basis functions.



Kernel Regression

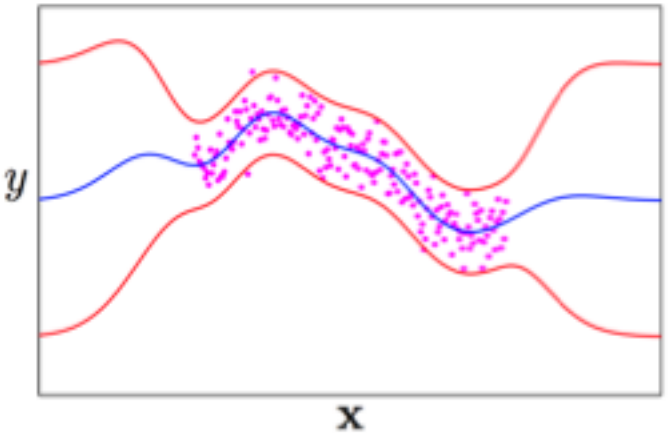
- So far the kernel was defined in terms of a finite number of basis functions $\Phi(x)$
- We can eliminate the concept of the basis functions and work simply with kernels
- Nadaraya-Watson regression $$\widehat{m}_h(x) = \frac{\sum_{i=1}^{n} K_h(x - x_i) y_i}{\sum_{i=1}^{n} K_h(x - x_i)}$$
- We want to estimate $y(x) = h(x)$: we use points close to x weighted by some function of the distance $K_h(x-x_i)$: as the distance increases the weights drop off
- Kernel K_h does not have to be a covariance matrix, but if it is then this becomes a gaussian process
- Why a matrix? Because if there are a bunch of data points x_i close to each other they should count as a single point (all give equal information). This is ignored in N-W regression

Gaussian Process

- We interpret the kernel as $K_{ij} = \mathrm{Cov}(y(x_i), y(x_i))$ and define $y(x)$ as a random variable with a multi-variate gaussian distribution $N(\mu,K)$
- 2-variables

$$\mu = \begin{bmatrix} \mu(x) \\ \mu(x') \end{bmatrix} \quad \Sigma = \begin{bmatrix} K(x,x) & K(x,x') \\ K(x',x) & K(x',x') \end{bmatrix}$$

- We then use posterior prediction for y: we get both the mean m and variance $K^{1/2}$
- We can interpret GP as regression on an infinite basis
- Smoothness versus sparseness



Gaussian Process

- Example covariance function K for translational and rotational invariant case

$$K(x_i, x_j) = v_0 \exp\left\{-\left(\frac{|x_i - x_j|}{r}\right)^{\alpha}\right\} + v_1 + v_2\,\delta_{ij}$$

- Kernel parameters can be learned from data using optimization

v_0	signal variance
v_1	variance of bias
v_2	noise variance
r	lengthscale
α	roughness

GP for Regression

- Model $\mathcal{D} = \{(\mathbf{x}_i, y_i)_{i=1}^n\} = (\mathbf{X}, \mathbf{y})$

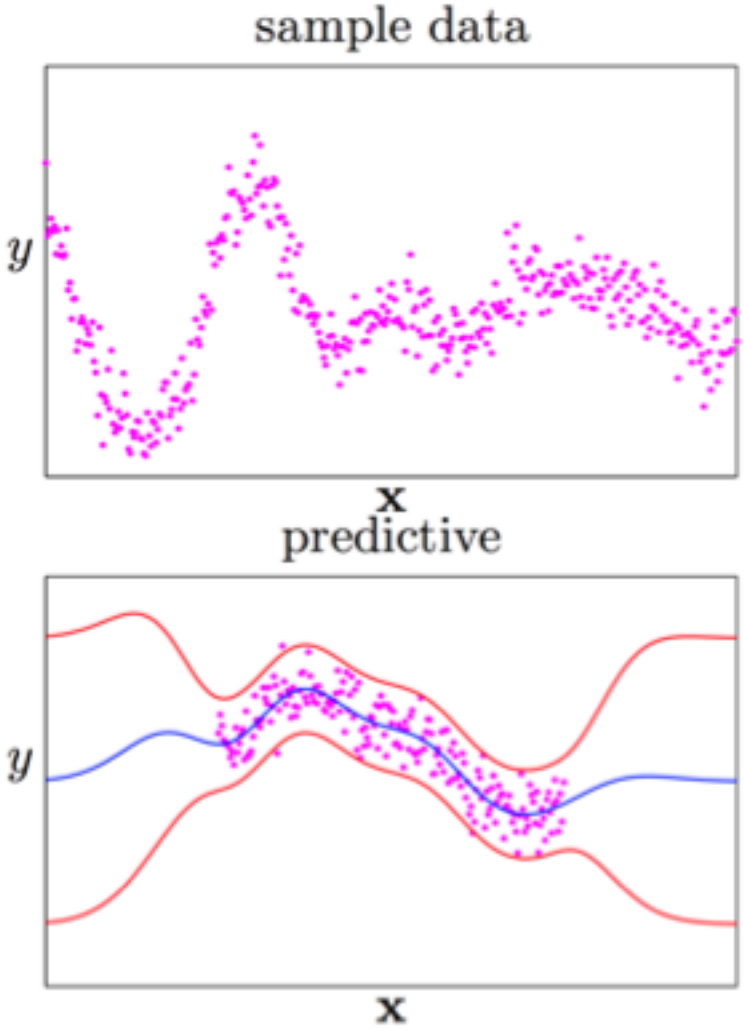
$$\begin{aligned} y_i &= f(\mathbf{x}_i) + \epsilon_i \\ f &\sim \mathsf{GP}(\cdot|0, K) \\ \epsilon_i &\sim \mathsf{N}(\cdot|0, \sigma^2) \end{aligned}$$

- We can marginalize over f

$$p(y_*|\mathbf{x}_*, \mathcal{D}) = \int p(y_*|\mathbf{x}_*, f, \mathcal{D})\, p(f|\mathcal{D})\, df$$

GP Regression

Gaussian observation noise: $y_n = f_n + \epsilon_n$, where $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$



marginal likelihood

$$p(\mathbf{y}|\mathbf{X}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_N + \sigma^2\mathbf{I})$$

predictive distribution

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

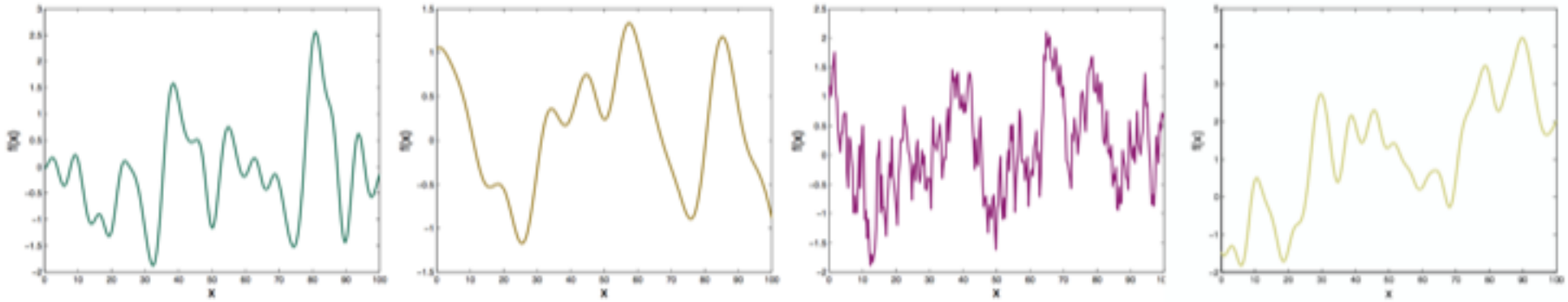
$$\mu_* = \mathbf{K}_{*N}(\mathbf{K}_N + \sigma^2\mathbf{I})^{-1}\mathbf{y}$$

$$\sigma_*^2 = K_{**} - \mathbf{K}_{*N}(\mathbf{K}_N + \sigma^2\mathbf{I})^{-1}\mathbf{K}_{N*} + \sigma^2$$

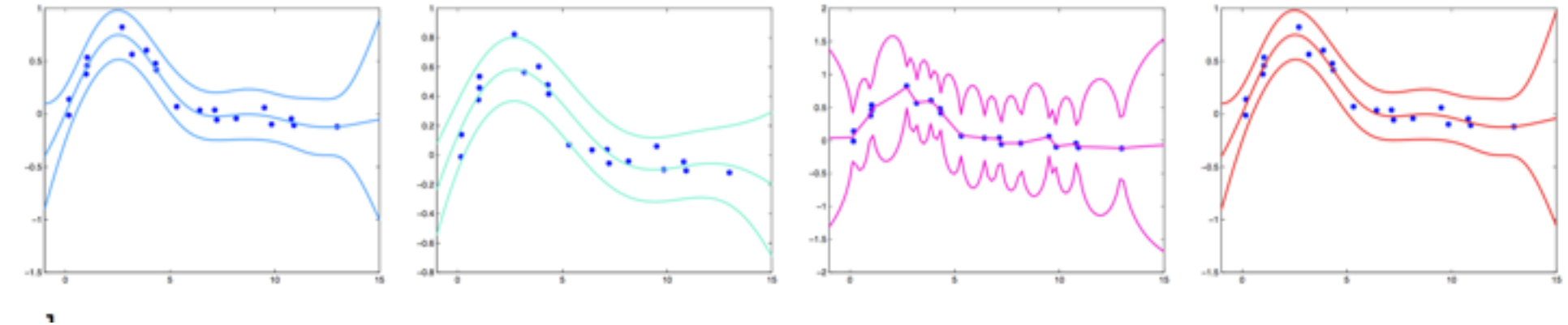
This handles properly even when points are not uniform

Predictions for different kernels

A sample from the prior for each covariance function:



Corresponding predictions, mean with two standard deviations:



Learning the Kernel

$$K_{\boldsymbol{\theta}}(\mathbf{x}_i, \mathbf{x}_j) = v_0 \exp\left\{ -\sum_{d=1}^{D} \left(\frac{|x_i^{(d)} - x_j^{(d)}|}{r_d} \right)^{\alpha} \right\} + v_1$$

$$\boldsymbol{\theta} = (v_0, v_1, r_1, \ldots, r_d, \alpha)$$

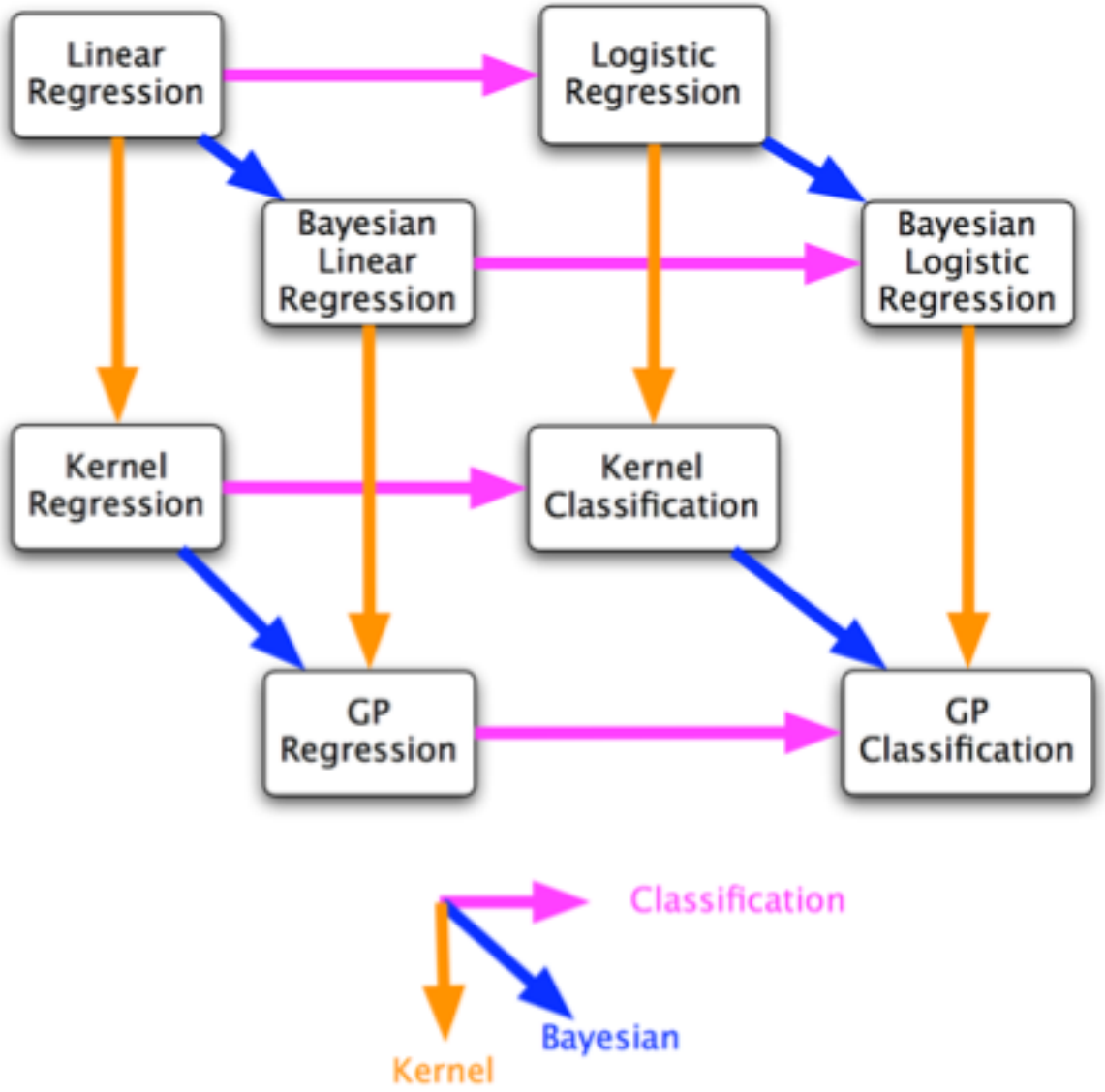
$$\ln p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = -\frac{1}{2} \ln \det(\mathbf{K}_{\boldsymbol{\theta}} + \sigma^2 \mathbf{I}) - \frac{1}{2} \mathbf{y}^{\top} (\mathbf{K}_{\boldsymbol{\theta}} + \sigma^2 \mathbf{I})^{-1} \mathbf{y} + \text{const}$$

- This can be viewed as a likelihood of θ given the data *(x,y)*
- Bayesian view: kernel parameters are hyperpriors and we want to determine them from the data
- We can use NL optimization to determine the posterior of θ (or just MAP)

From Linear Regression to GP

- We started with a linear regression with inputs x_i and noisy y_i: $y_i = a + b x_i + \varepsilon_i$
- We generalized this to a general basis with M basis functions $y_i = \Sigma_{j=1}^{M} a_j \phi(x_i) + \varepsilon_i$
- Next we performed Bayesian regression by adding a gaussian prior on coefficients $a_j = N(0, \lambda_j)$
- This is equivalent to regularization adding L2 norm and minimize $l = \Sigma_{i=1}^{N} [\Sigma_{j=1}^{M} a_j \phi(x_i) - y_i]^2 + \Sigma_{j=1}^{M} \lambda_j a_j^2$
- Next we marginalize over a_j: we are left with $E(y_i) = 0$ and $K_{ij} = Cov(y(x_i), y(x_j)) = \Sigma_{j=1}^{M} \lambda_j \phi(x_i) \phi(x_j)$
- This is a gaussian process with a finite number of basis functions.
- Many GP kernels correspond to infinite number of basis functions.
- We can remove the concept of basis and only work with GP kernels

Connections between regression/ classification models



Summary

- Interpolations: polynomial, spline, rational…
- They are just a subset of regression models, and one can connect them to regularized regression, which can be connected to Bayesian regression, which can be connected to kernel regression
- This can also be connected to classification, next lecture

Literature

- *Pattern Recognition and Machine Learning*, C. Bishop, Chapter 3
- *Bayesian Data Analysis,* Gelman et al. , Chapter 20-21
- http://www.gaussianprocess.org
- https://arxiv.org/pdf/1505.02965.pdf
- http://mlss2011.comp.nus.edu.sg/uploads/Site/lect1gp.pdf