LECTURE 11: From Interpolations to Regressions to Gaussian Processes

- 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

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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

(a)

(b)

2

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

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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:

$$y = Ay_j + By_{j+1} + Cy_j'' + Dy_{j+1}''$$

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

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)*
- 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 $n > m$

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

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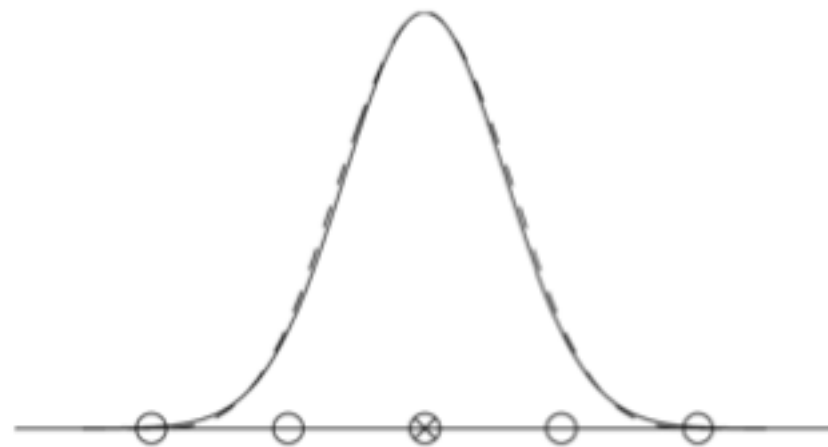
$$\mu(x) = \sum_{h=1}^{H} \beta_h b_h(x)$$

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

- Very close to gaussian

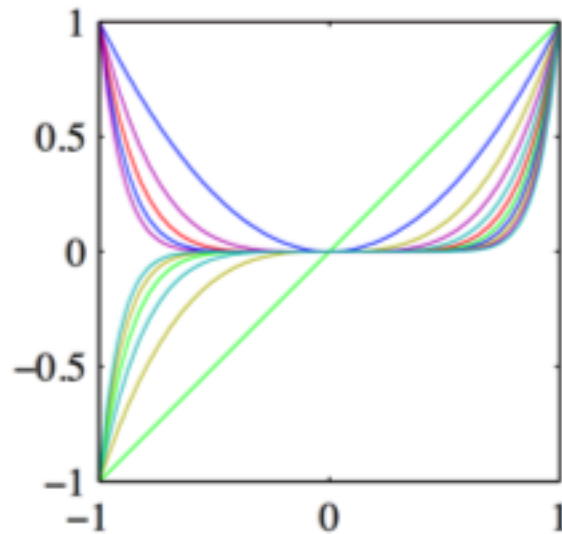$$b_h(x) = \exp\left(-\frac{|x - x_h|^2}{l^2}\right)$$

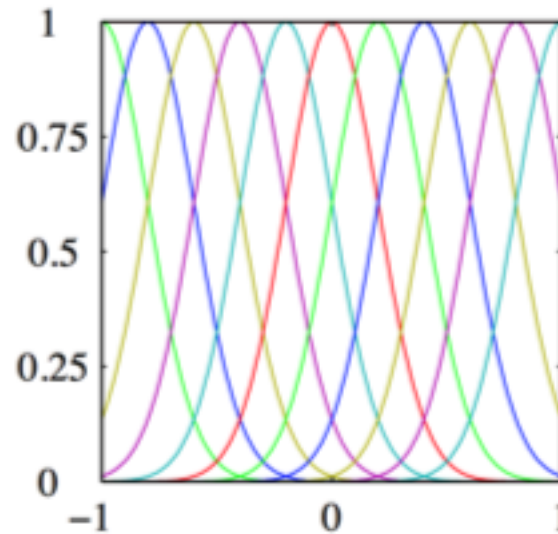- Gaussian is infinitely differentiable (i.e. smoother) but not sparse
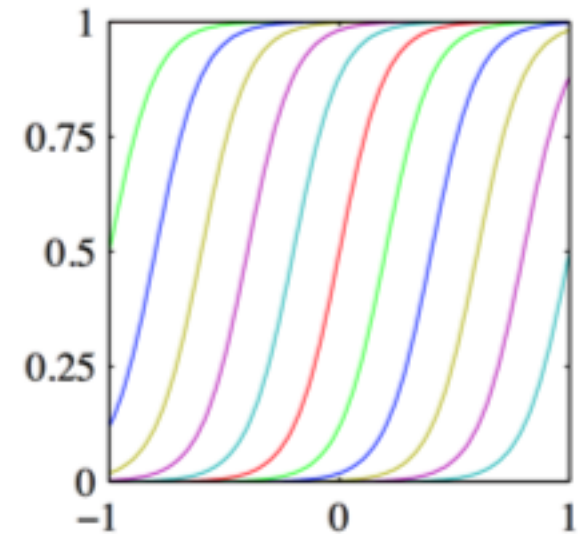
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Example of Basis Functions

- 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 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

High λ: low scatter, high bias,
Low λ : high scatter, low bias

Example:
 N = M = 25,
Gaussian
basis
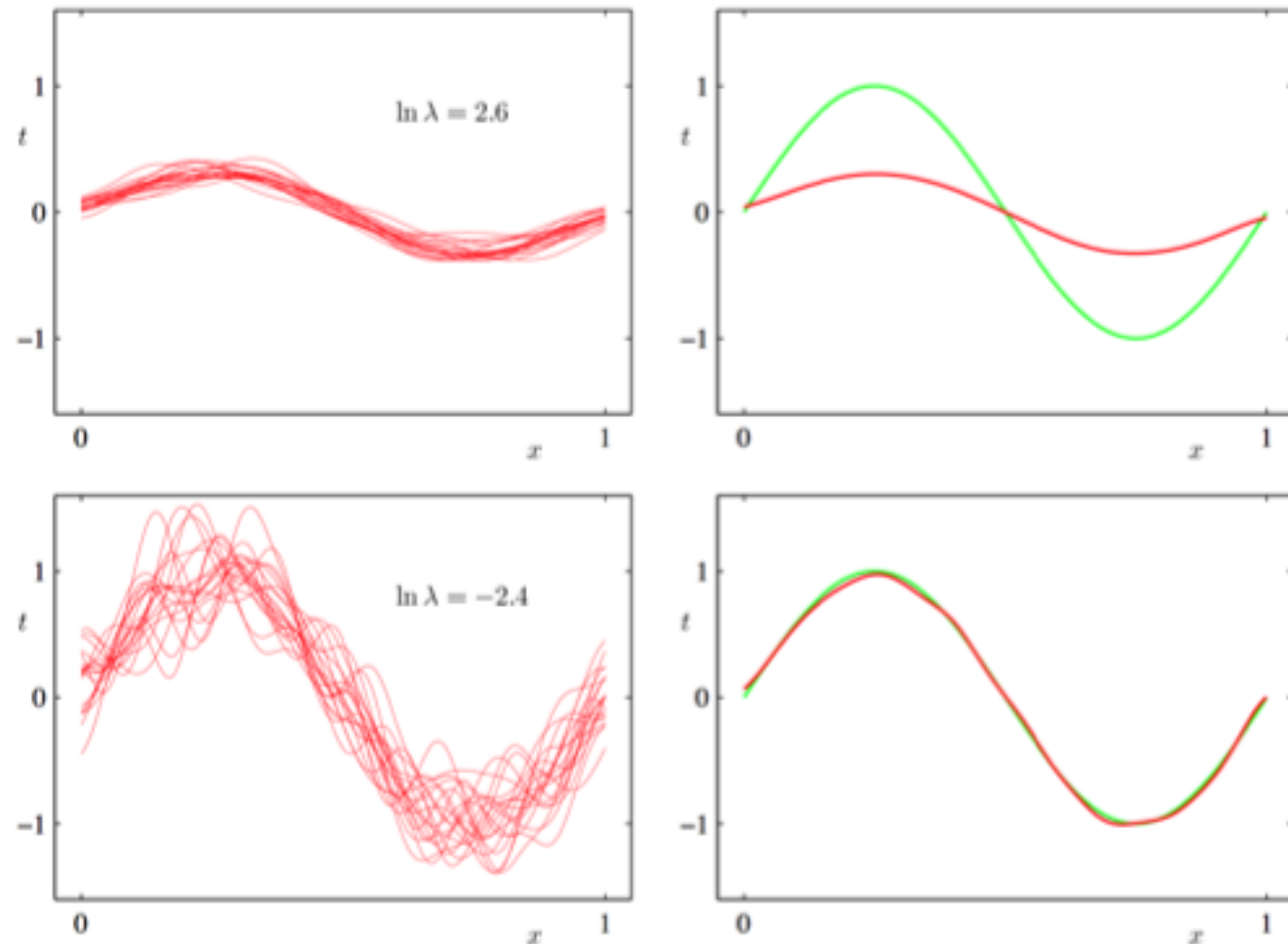
Bayesian Regression

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

- In the Bayesian context we perform regression of coefficients a_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 $\quad p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$

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

- Posterior
$$
\begin{aligned}
\mathbf{m}_N &= \mathbf{S}_N(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\Phi^{\mathrm{T}}\mathbf{t}) \\
\mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta\Phi^{\mathrm{T}}\Phi
\end{aligned}
$$

- We want to predict at arbitrary t:

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

Prediction for t

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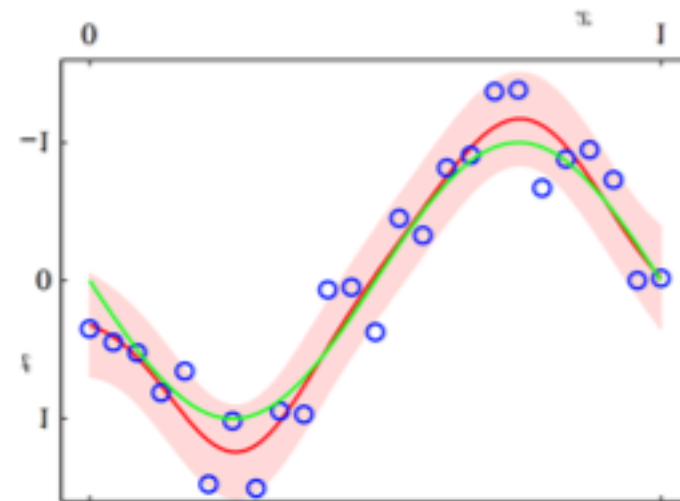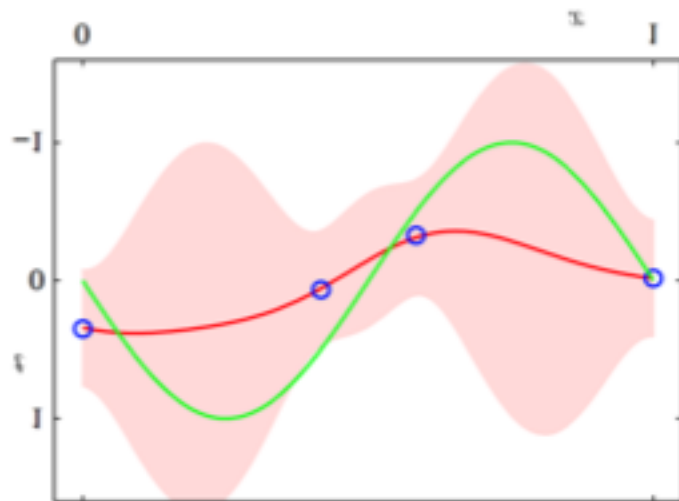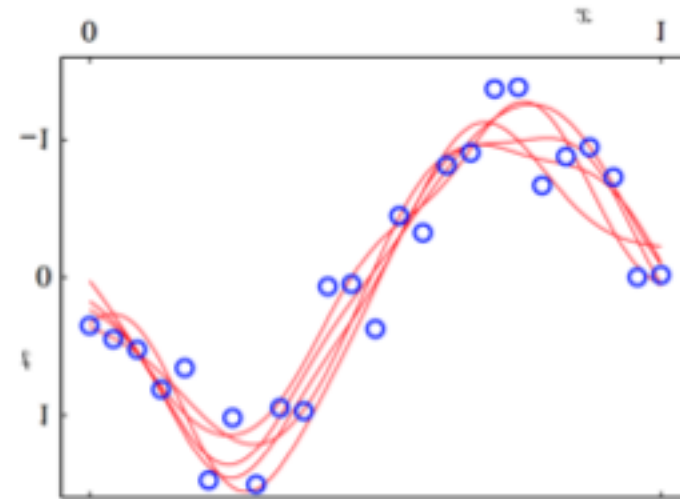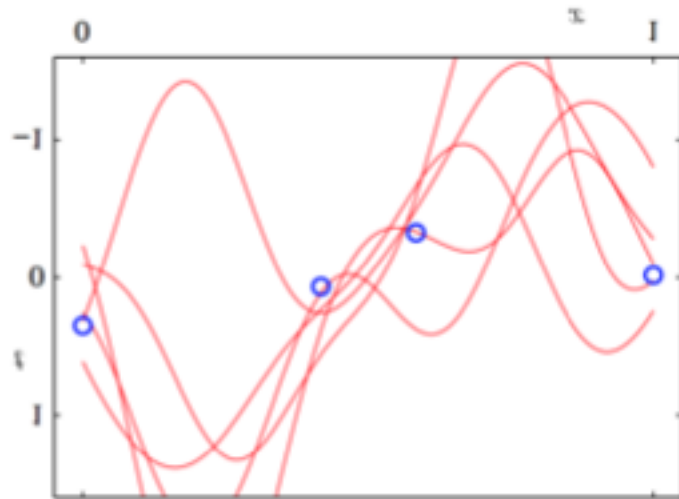
$$p(t|\mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

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

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

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

Examples

Kernel Picture

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

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

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

Basis functions $\longleftrightarrow$ kernel duality

With $\Psi(\mathbf{x}) = \beta^{-1/2}\mathbf{S}_N^{1/2}\Phi(\mathbf{x})$, $k(\mathbf{x}, \mathbf{x}') = \Psi(\mathbf{x})^{\mathrm{T}}\Psi(\mathbf{x}')$
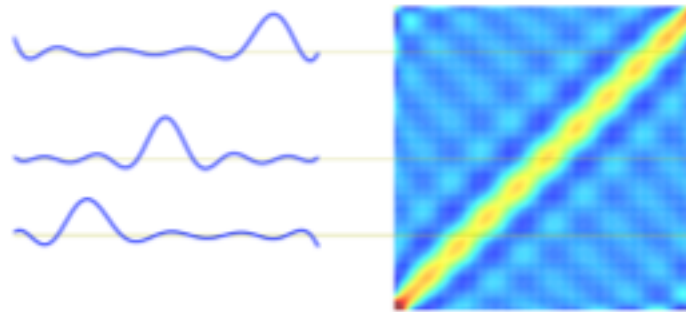
The kernel sums to one (over the training set)

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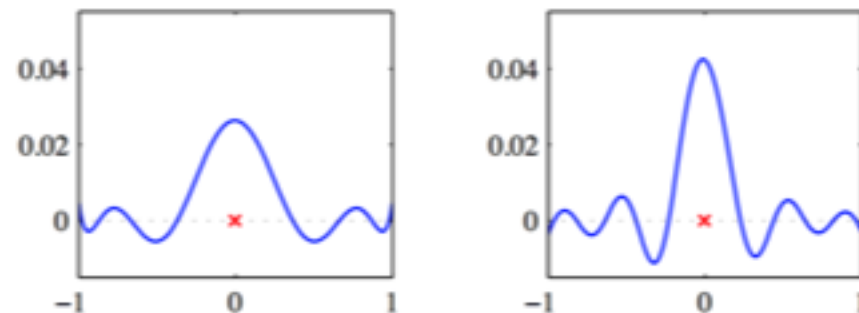
Kernel Examples

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 $K_h(x\text{-}x_i)$: as the distance increases the weights drop off

- Kernel K_h does not have to be a covariance function, but if it is then this becomes a gaussian process
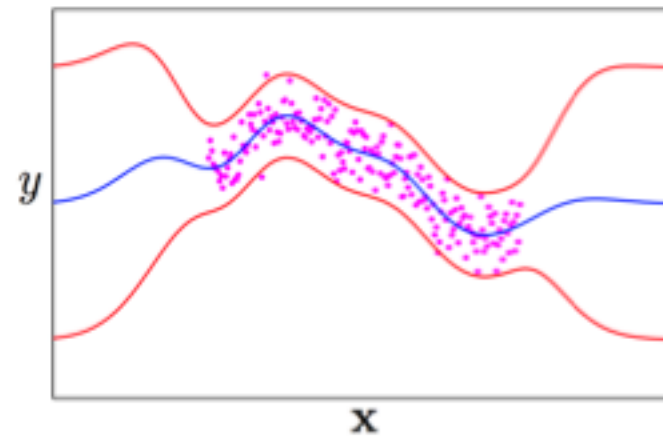
Gaussian Process

- We interpret the kernel as $K_{ij} = \text{Cov}(y(x_i), y(x_i))$ 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

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

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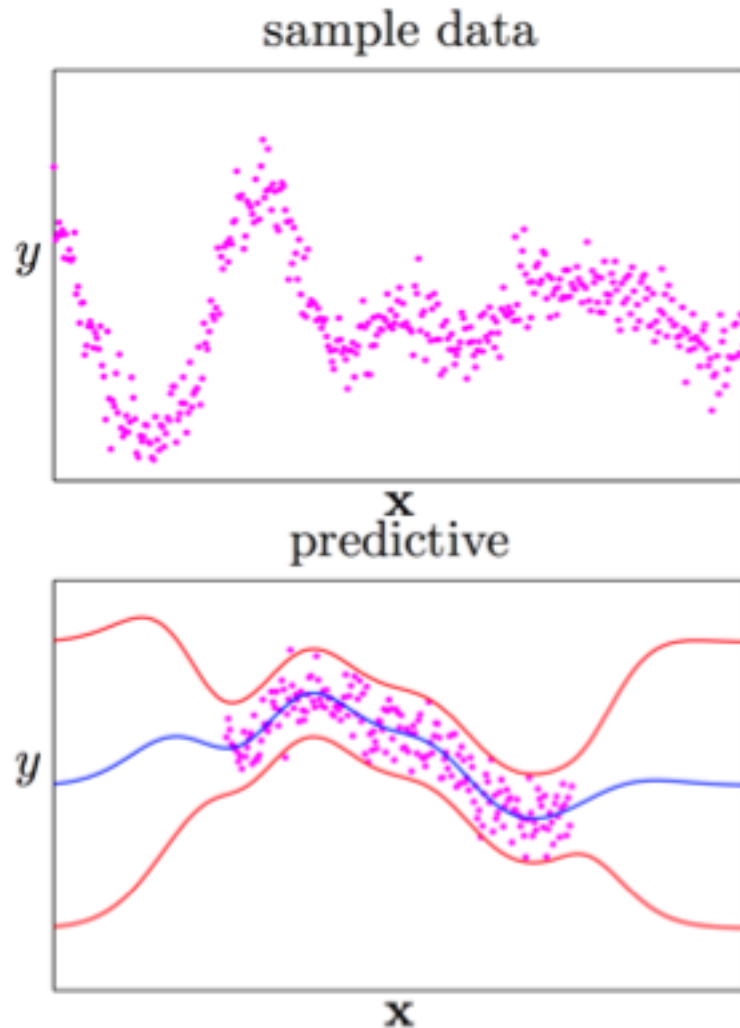f &\sim \mathsf{GP}(\cdot|0, K) \\
\epsilon_i &\sim \mathsf{N}(\cdot|0, \sigma^2)
\end{aligned}
$$

- 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 $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$

sample data

y

$\mathbf{x}$

predictive

y
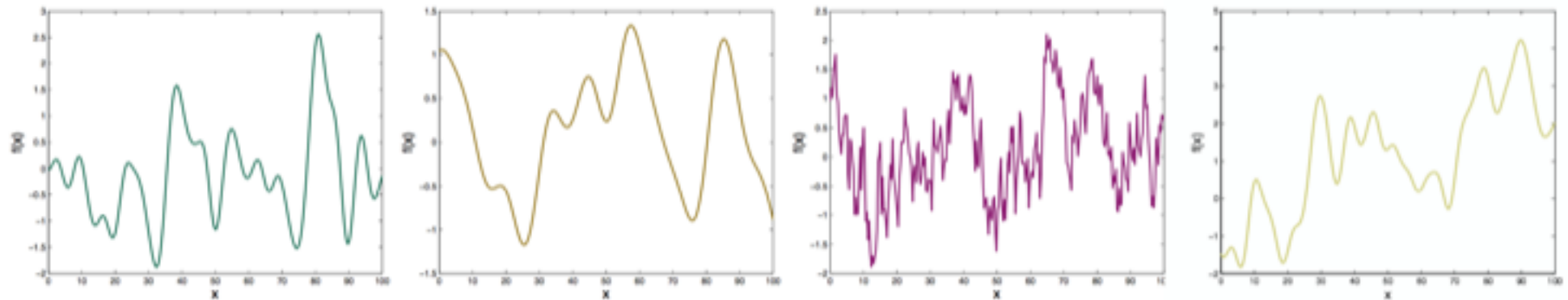
$\mathbf{x}$

marginal likelihood
$$p(\mathbf{y}|\mathbf{X}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_N + \sigma^2 \mathbf{I})$$
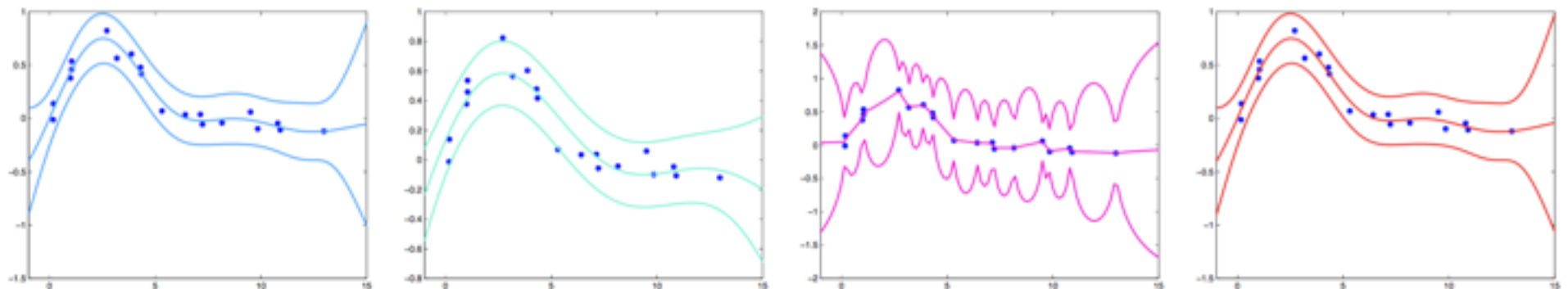
predictive distribution
$$p(y_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) = \mathcal{N}(\mu_*, \sigma_*^2)$$

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

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)*

- We can use NL optimization to determine MLE θ

From Linear Regression to GP

- We started with a linear regression with inputs x_i and noisy y_i:
$y_i = a + bx_i + \varepsilon_i$

- 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 adding L_2 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.

Connections between regression/ classification models
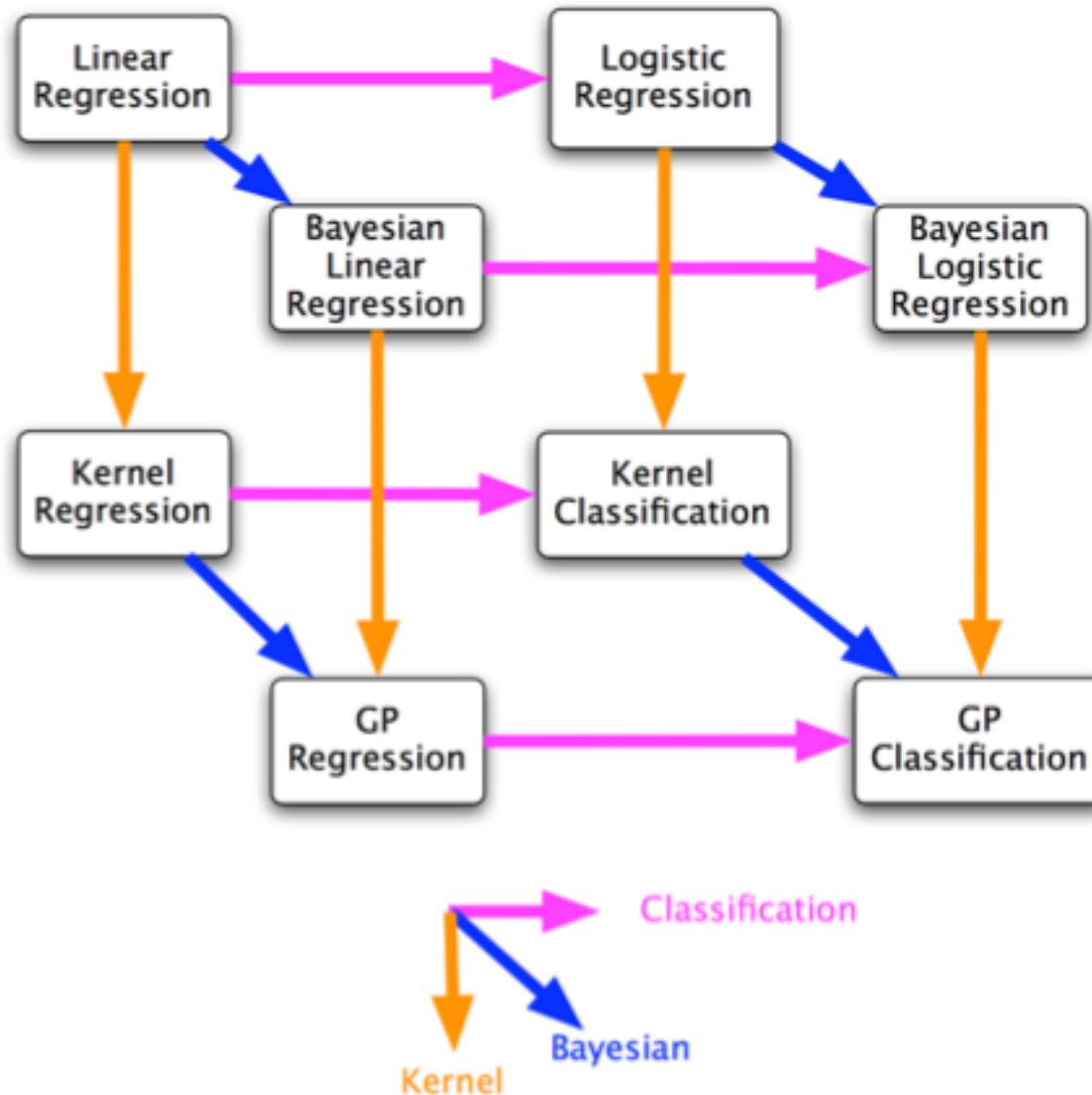
Summary

- 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

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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