Introduction to Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

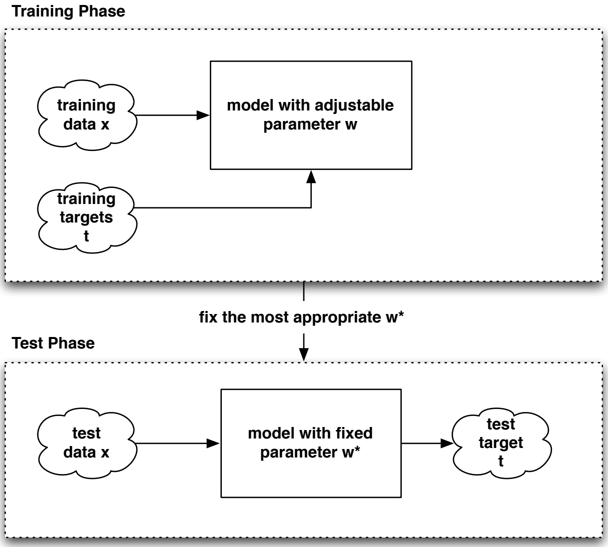
Part IV

Linear Regression 2

Linear Regression

- Basis functions
- Maximum Likelihood with Gaussian Noise
- Regularisation

Training and Testing



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Bayesian Regression

- Bayes Theorem

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{normalisation}} \qquad p(\mathbf{w} \mid \mathbf{t}) = \frac{p(\mathbf{t} \mid \mathbf{w})\, p(\mathbf{w})}{p(\mathbf{t})}$$

  where we left out the conditioning on $\mathbf{x}$ (always assumed), and β, which is assumed to be constant.
- likelihood for i.i.d. data (β, inverse variance of noise)

$$\begin{aligned} p(\mathbf{t} \mid \mathbf{w}) &= \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}) \\ &= \prod_{n=1}^{N} \mathcal{N}(t_n \mid \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}) \\ &= \text{const} \times \exp\{-\beta \frac{1}{2} (\mathbf{t} - \boldsymbol{\Phi}\mathbf{w})^T (\mathbf{t} - \boldsymbol{\Phi}\mathbf{w})\} \\ &= \mathcal{N}(\mathbf{t} \mid \boldsymbol{\Phi}\mathbf{w}, \beta^{-1}\mathbf{I}) \end{aligned}$$

How to choose a prior?

- Can we find a prior for the given likelihood which
  - makes sense for the problem at hand
  - allows us to find a posterior in a 'nice' form

An answer to the second question:

Definition (Conjugate Prior)

A class of prior probability distributions $p(w)$ is conjugate to a class of likelihood functions $p(x \mid w)$ if the resulting posterior distributions $p(w \mid x)$ are in the same family as $p(w)$.

Examples of Conjugate Prior Distributions

Table: Discrete likelihood distributions

Likelihood	Conjugate Prior
Bernoulli	Beta
Binomial	Beta
Poisson	Gamma
Multinomial	Dirichlet

Table: Continuous likelihood distributions

Likelihood	Conjugate Prior
Uniform	Pareto
Exponential	Gamma
Normal	Normal
Multivariate normal	Multivariate normal

Conjugate Prior to a Gaussian Distribution

- Example : The Gaussian family is conjugate to itself with respect to a Gaussian likelihood function: if the likelihood function is Gaussian, choosing a Gaussian prior will ensure that the posterior distribution is also Gaussian.
- Given a marginal distribution for $\mathbf{x}$ and a conditional Gaussian distribution for $\mathbf{y}$ given $\mathbf{x}$ in the form

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \,|\, \boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$$
$$p(\mathbf{y} \,|\, \mathbf{x}) = \mathcal{N}(\mathbf{y} \,|\, \boldsymbol{A}x + \mathbf{b}, \boldsymbol{L}^{-1})$$

- we get

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \,|\, \boldsymbol{A}\boldsymbol{\mu} + \mathbf{b}, \boldsymbol{L}^{-1} + \boldsymbol{A}\boldsymbol{\Lambda}^{-1}\boldsymbol{A}^T)$$
$$p(\mathbf{x} \,|\, \mathbf{y}) = \mathcal{N}(\mathbf{x} \,|\, \boldsymbol{\Sigma}\{\boldsymbol{A}^T\boldsymbol{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\}, \boldsymbol{\Sigma})$$

where $\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \boldsymbol{A}^T\boldsymbol{L}\boldsymbol{A})^{-1}$.

Bayesian Regression

- Choose a Gaussian prior with mean $\mathbf{m}_0$ and covariance $\mathbf{S}_0$

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

- After having seen N training data pairs $(\mathbf{x}_n, t_n)$, the posterior for the given likelihood is now

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

where

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

- The posterior is Gaussian, therefore mode $=$ mean.
- The maximum posterior weight vector $\mathbf{w}_{MAP} = \mathbf{m}_N$.
- Assume infinitely broad prior $\mathbf{S}_0 = \alpha^{-1}\mathbf{I}$ with $\alpha \to 0$, the mean reduces to the maximum likelihood $\mathbf{w}_{ML}$.

Bayesian Regression

- If we have not yet seen any data point ($N = 0$), the posterior is equal to the prior.
- Sequential arrival of data points : Each posterior distribution calculated after the arrival of a data point and target value, acts as the prior distribution for the subsequent data point.
- Nicely fits a sequential learning framework.

Bayesian Regression

- Special simplified prior in the remainder, $\mathbf{m}_0 = 0$ and $\mathbf{S}_0 = \alpha^{-1}\mathbf{I}$,

$$p(\mathbf{x} \mid \alpha) = \mathcal{N}(\mathbf{x} \mid 0, \alpha^{-1}\mathbf{I})$$

- The parameters of the posterior distribution $p(\mathbf{w} \mid \mathbf{t}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_N, \mathbf{S}_N)$ are now

$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^T \mathbf{t}$$
$$\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}$$

- For $\alpha \to 0$ we get

$$\mathbf{m}_N \to \mathbf{w}_{ML} = (\mathbf{\Phi}^T \mathbf{\Phi})^{-1} \mathbf{\Phi}^T \mathbf{t}$$

- Log of posterior is sum of log likelihood and log of prior

$$\ln p(\mathbf{w} \mid \mathbf{t}) = -\frac{\beta}{2}(\mathbf{t} - \mathbf{\Phi}\mathbf{w})^T(\mathbf{t} - \mathbf{\Phi}\mathbf{w}) - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const}$$

Bayesian Regression

- Log of posterior is sum of log likelihood and log of prior

$$\ln p(\mathbf{w} \,|\, \mathbf{t}) = -\,\beta \underbrace{\frac{1}{2}(\mathbf{t} - \mathbf{\Phi w})^T(\mathbf{t} - \mathbf{\Phi w})}_{\text{sum-of-squares-error}}$$

$$-\,\frac{\alpha}{2} \underbrace{\mathbf{w}^T\mathbf{w}}_{\text{quadr. regulariser}} + \text{const}$$

- Maximising the posterior distribution with respect to $\mathbf{w}$ corresponds to minimising the sum-of-squares error function with the addition of a quadratic regularisation term $\lambda = \alpha/\beta$.

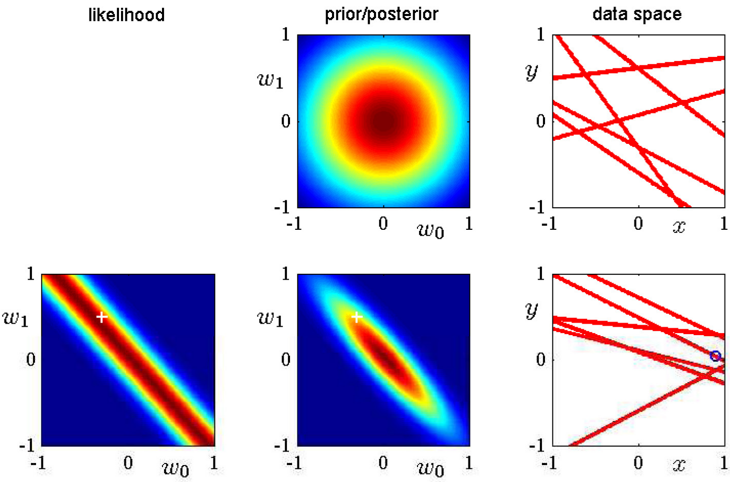
Sequential Update of the Posterior

- Example of a linear basis function model
- Single input x, single output t
- Linear model $y(x, \mathbf{w}) = w_0 + w_1 x$.
- Data creation
  1. Choose an x_n from the uniform distribution $\mathcal{U}(x \mid -1, 1)$.
  2. Calculate $f(x_n, \mathbf{a}) = a_0 + a_1 x_n$, where $a_0 = -0.3$, $a_1 = 0.5$.
  3. Add Gaussian noise with standard deviation $\sigma = 0.2$,

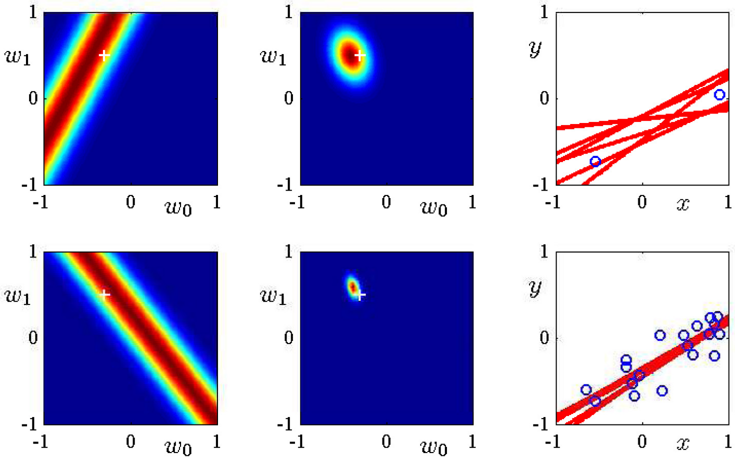
$$t_n = \mathcal{N}(x_n \,|\, f(x_n, \mathbf{a}), 0.04)$$

- Set the precision of the uniform prior to $\alpha = 2.0$.

Sequential Update of the Posterior



Sequential Update of the Posterior



Predictive Distribution

- In the training phase, data $\mathbf{x}$ and targets $\mathbf{t}$ are provided
- In the test phase, a new data value x is given and the corresponding target value t is asked for
- Bayesian approach: Find the probability of the test target t given the test data x, the training data $\mathbf{x}$ and the training targets $\mathbf{t}$

$$p(t \mid x, \mathbf{x}, \mathbf{t})$$

- This is the Predictive Distribution.

How to calculate the Predictive Distribution?

- Introduce the model parameter $\mathbf{w}$ via the sum rule

$$
\begin{aligned}
p(t \mid x, \mathbf{x}, \mathbf{t}) &= \int p(t, \mathbf{w} \mid x, \mathbf{x}, \mathbf{t}) d\mathbf{w} \\
&= \int p(t \mid \mathbf{w}, x, \mathbf{x}, \mathbf{t}) p(\mathbf{w} \mid x, \mathbf{x}, \mathbf{t}) d\mathbf{w}
\end{aligned}
$$

- The test target t depends only on the test data x and the model parameter $\mathbf{w}$, but not on the training data and the training targets

$$p(t \mid \mathbf{w}, x, \mathbf{x}, \mathbf{t}) = p(t \mid \mathbf{w}, x)$$

- The model parameter $\mathbf{w}$ are learned with the training data $\mathbf{x}$ and the training targets $\mathbf{t}$ only

$$p(\mathbf{w} \mid x, \mathbf{x}, \mathbf{t}) = p(\mathbf{w} \mid \mathbf{x}, \mathbf{t})$$

- Predictive Distribution

$$p(t \mid x, \mathbf{x}, \mathbf{t}) = \int p(t \mid \mathbf{w}, x) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) d\mathbf{w}$$

Proof of the Predictive Distribution

- How to prove the Predictive Distribution in the general form?

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

- Convert each conditional probability on the right-hand-side into a joint probability.

$$\begin{aligned}
&\int p(t \,|\, \mathbf{w}, x, \mathbf{x}, \mathbf{t}) p(\mathbf{w} \,|\, x, \mathbf{x}, \mathbf{t}) d\mathbf{w} \\
&= \int \frac{p(t, \mathbf{w}, x, \mathbf{x}, \mathbf{t})}{p(\mathbf{w}, x, \mathbf{x}, \mathbf{t})} \frac{p(\mathbf{w}, x, \mathbf{x}, \mathbf{t})}{p(x, \mathbf{x}, \mathbf{t})} d\mathbf{w} \\
&= \int \frac{p(t, \mathbf{w}, x, \mathbf{x}, \mathbf{t})}{p(x, \mathbf{x}, \mathbf{t})} d\mathbf{w} \\
&= \frac{p(t, x, \mathbf{x}, \mathbf{t})}{p(x, \mathbf{x}, \mathbf{t})} \\
&= p(t \,|\, x, \mathbf{x}, \mathbf{t})
\end{aligned}$$

Predictive Distribution with Simplified Prior

- Find the predictive distribution

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

(remember : The conditioning on the input variables $\mathbf{x}$ is often suppressed to simplify the notation.)

- Now we know

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid \mathbf{w}^T \phi(\mathbf{x}_n), \beta^{-1})$$

- and the posterior was

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

where

$$\begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \mathbf{\Phi}^T \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi} \end{aligned}$$

Predictive Distribution with Simplified Prior

- If we do the convolution of the two Gaussians, we get for the predictive distribution

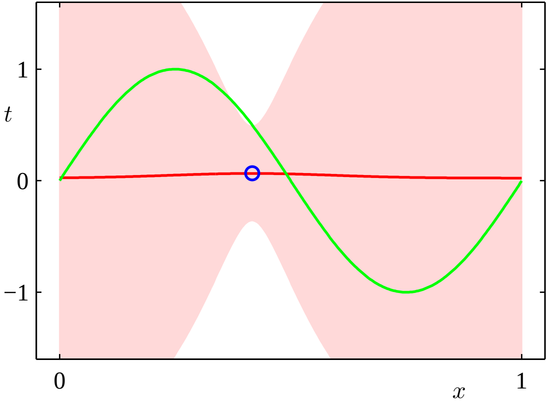
$$p(t \mid \mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t \mid \mathbf{m}_N^T \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

where the variance $\sigma_N^2(\mathbf{x})$ is given by

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}).$$

Predictive Distribution with Simplified Prior

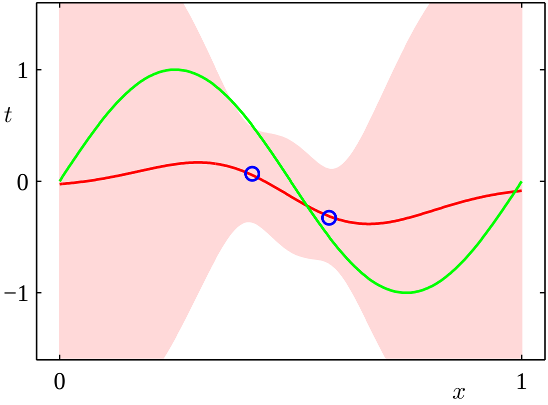
Example with artificial sinusoidal data from $\sin(2\pi x)$ (green) and added noise. Number of data points $N = 1$.



Mean of the predictive distribution (red) and regions of one standard deviation from mean (red shaded).

Predictive Distribution with Simplified Prior

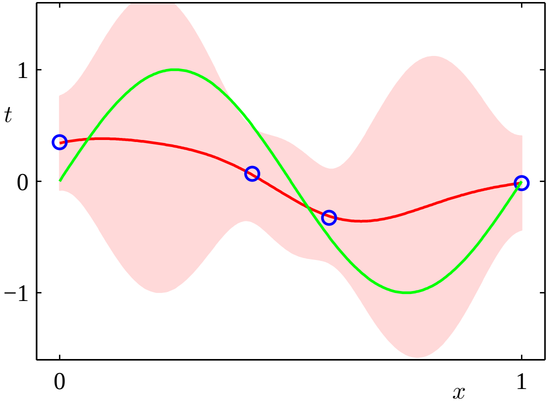
Example with artificial sinusoidal data from $\sin(2\pi x)$ (green) and added noise. Number of data points $N = 2$.



Mean of the predictive distribution (red) and regions of one standard deviation from mean (red shaded).

Predictive Distribution with Simplified Prior

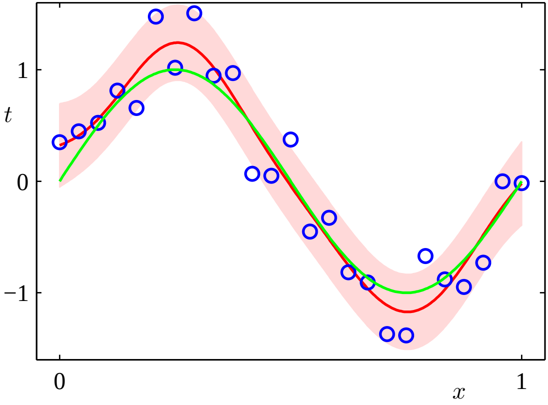
Example with artificial sinusoidal data from $\sin(2\pi x)$ (green) and added noise. Number of data points $N = 4$.



Mean of the predictive distribution (red) and regions of one standard deviation from mean (red shaded).

Predictive Distribution with Simplified Prior

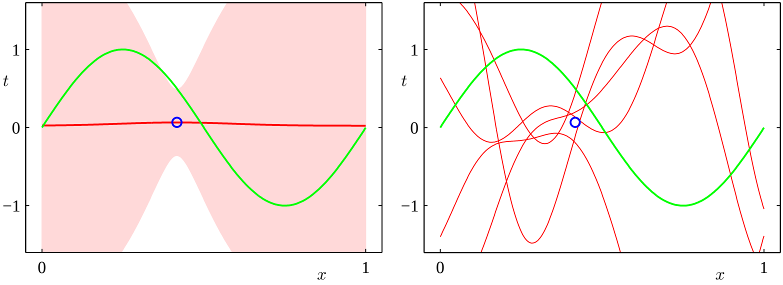
Example with artificial sinusoidal data from $\sin(2\pi x)$ (green) and added noise. Number of data points $N = 25$.



Mean of the predictive distribution (red) and regions of one standard deviation from mean (red shaded).

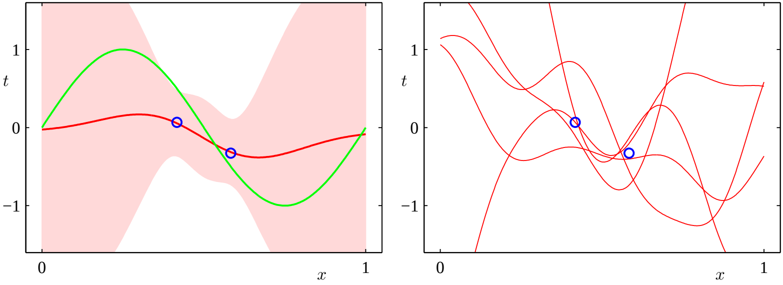
Predictive Distribution with Simplified Prior

Plots of the function $y(x, \mathbf{w})$ using samples from the posterior distribution over $\mathbf{w}$. Number of data points $N = 1$.



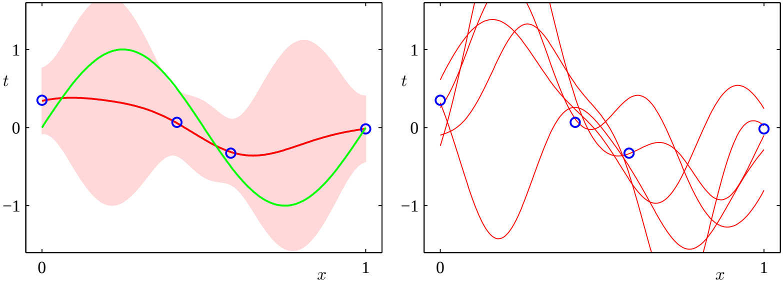
Predictive Distribution with Simplified Prior

Plots of the function $y(x, \mathbf{w})$ using samples from the posterior distribution over $\mathbf{w}$. Number of data points $N = 2$.



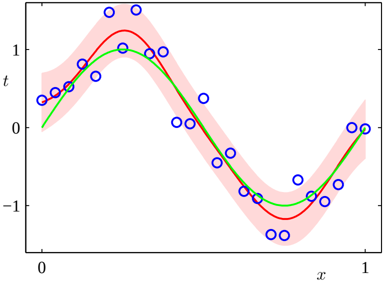
Predictive Distribution with Simplified Prior

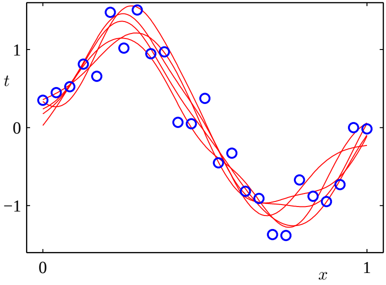
Plots of the function $y(x, \mathbf{w})$ using samples from the posterior distribution over $\mathbf{w}$. Number of data points $N = 4$.



Predictive Distribution with Simplified Prior

Plots of the function $y(x, \mathbf{w})$ using samples from the posterior distribution over $\mathbf{w}$. Number of data points $N = 25$.





Limitations of Linear Basis Function Models

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- Basis function $\phi_j(\mathbf{x})$ are fixed before the training data set is observed.
- Curse of dimensionality : Number of basis function grows rapidly, often exponentially, with the dimensionality D.
- But typical data sets have two nice properties which can be exploited if the basis functions are not fixed :
    - Data lie close to a nonlinear manifold with intrinsic dimension much smaller than D. Need algorithms which place basis functions only where data are (e.g. radial basis function networks, support vector machines, relevance vector machines, neural networks).
    - Target variables may only depend on a few significant directions within the data manifold. Need algorithms which can exploit this property (Neural networks).

Curse of Dimensionality

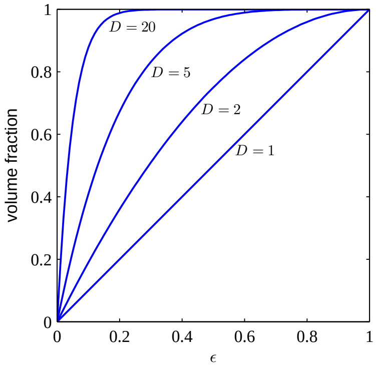
- Linear Algebra allows us to operate in n-dimensional vector spaces using the intution from our 3-dimensional world as a vector space. No surprises as long as n is finite.
- If we add more structure to a vector space (e.g. inner product, metric), our intution gained from the 3-dimensional world around us may be wrong.
- Example: Sphere of radius $r = 1$. What is the fraction of the volume of the sphere in a D-dimensional space which lies between radius $r = 1$ and $r = 1 - \epsilon$?
- Volume scales like r^D, therefore the formula for the volume of a sphere is $V_D(r) = K_D r^D$.

$$\frac{V_D(1) - V_D(1-\epsilon)}{V_D(1)} = 1 - (1-\epsilon)^D$$

Curse of Dimensionality

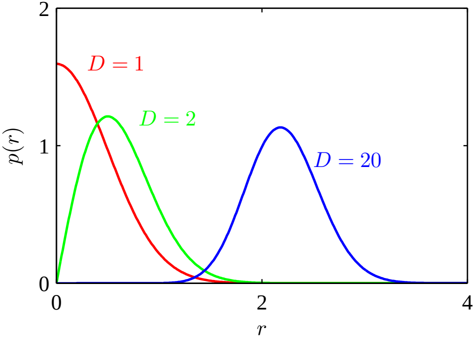
- Fraction of the volume of the sphere in a D-dimensional space which lies between radius $r = 1$ and $r = 1 - \epsilon$

$$\frac{V_D(1) - V_D(1-\epsilon)}{V_D(1)} = 1 - (1-\epsilon)^D$$



Curse of Dimensionality

- Probability density with respect to radius r of a Gaussian distribution for various values of the dimensionality D.



Curse of Dimensionality

- Probability density with respect to radius r of a Gaussian distribution for various values of the dimensionality D.
- Example: $D = 2$; assume $\mu = 0, \Sigma = I$

$$\mathcal{N}(x \,|\, 0, I) = \frac{1}{2\pi} \exp\left\{-\frac{1}{2} x^T x\right\} = \frac{1}{2\pi} \exp\left\{-\frac{1}{2}(x_1^2 + x_2^2)\right\}$$

- Coordinate transformation

$$x_1 = r\cos(\phi) \qquad x_2 = r\sin(\phi)$$

- Probability in the new coordinates

$$p(r, \phi \,|\, 0, I) = \mathcal{N}(r(x), \phi(x) \,|\, 0, I) \,|\, J \,|$$

where $|\, J \,| = r$ is the determinant of the Jacobian for the given coordinate transformation.

$$p(r, \phi \,|\, 0, I) = \frac{1}{2\pi} r \exp\left\{-\frac{1}{2} r^2\right\}$$

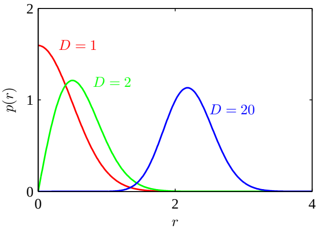
Curse of Dimensionality

- Probability density with respect to radius r of a Gaussian distribution for $D = 2$ (and $\mu = 0, \Sigma = I$)

$$p(r, \phi \,|\, 0, I) = \frac{1}{2\pi} r \exp\left\{-\frac{1}{2} r^2\right\}$$

- Integrate over all angles ϕ

$$p(r \,|\, 0, I) = \int_0^{2\pi} \frac{1}{2\pi} r \exp\left\{-\frac{1}{2} r^2\right\} d\phi = r \exp\left\{-\frac{1}{2} r^2\right\}$$



Summary: Linear Regression

- Basis functions
- Maximum likelihood with Gaussian noise
- Regularisation
- Bayesian linear regression
- Conjugate prior
- Sequential update of the posterior
- Predictive distribution
- Curse of dimensionality