Linear Models for Regression

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Topics in Linear Regression

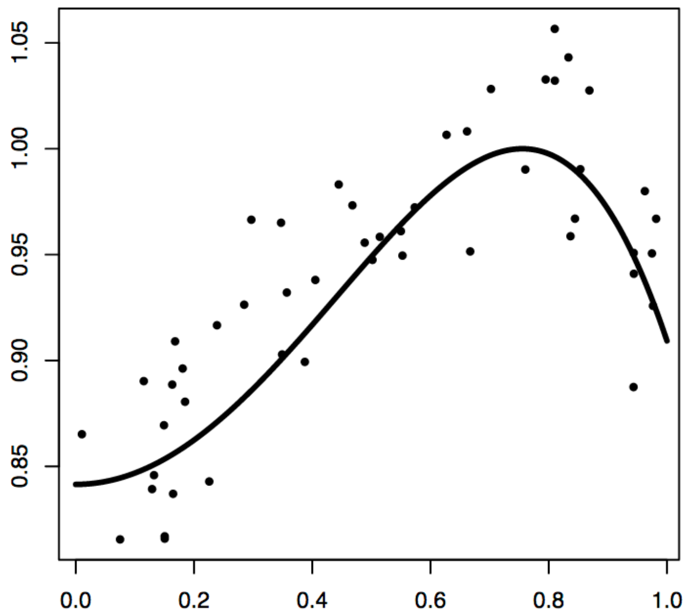
- What is regression?
  - Polynomial Curve Fitting with Scalar input
  - Linear Basis Function Models
- Maximum Likelihood and Least Squares
- Stochastic Gradient Descent
- Regularized Least Squares

The regression task

- It is a supervised learning task
- Goal of regression:
  - predict value of one or more target variables t
  - given d-dimensional vector x of input variables
  - With dataset of known inputs and outputs
    - $(\mathrm{x}_1,\mathrm{t}_1), ..(\mathrm{x}_N,\mathrm{t}_N)$
    - Where x_i is an input (possibly a vector) known as the predictor
    - t_i is the target output (or response) for case i which is real-valued
  - Goal is to predict t from x for some future test case
    - We are not trying to model the distribution of x
  - We dont expect predictor to be a linear function of x
    - So ordinary linear regression of inputs will not work
    - We need to allow for a nonlinear function of x
    - We don't have a theory of what form this function to take

An example problem

- Fifty points generated
  - With x uniform from $(0,1)$
  - y generated from formula $y=\sin(1+x^2)+\text{noise}$
    - Where noise has $N(0,0.03^2)$ distribution
    - Noise-free true function and data points are as shown



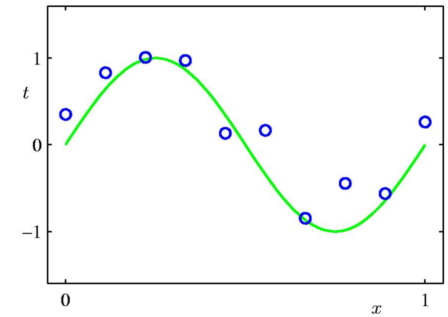
Application of Regression

- Expected claim amount an insured person will make (used to set insurance premiums) or prediction of future prices of securities
  - Also used for algorithmic trading

ML Terminology

- Regression
  - Predict a numerical value t given some input
    - Learning algorithm has to output function $f: \mathrm{R}^n \rightarrow \mathrm{R}$
      - where $n =$no of input variables
- Classification
  - If t value is a label (categories): $f: \mathrm{R}^n \rightarrow \{1,..,k\}$
- Ordinal Regression
  - Discrete values, ordered categories

Polynomial Curve Fitting with a Scalar



– With a single input variable x

– $y(x,\mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$

Training data set
N=10, Input x, target t

M is the order of the polynomial,

x^j denotes x raised to the power j,

Coefficients $w_0,\ldots,w_M$ are collectively denoted by vector $\mathbf{w}$

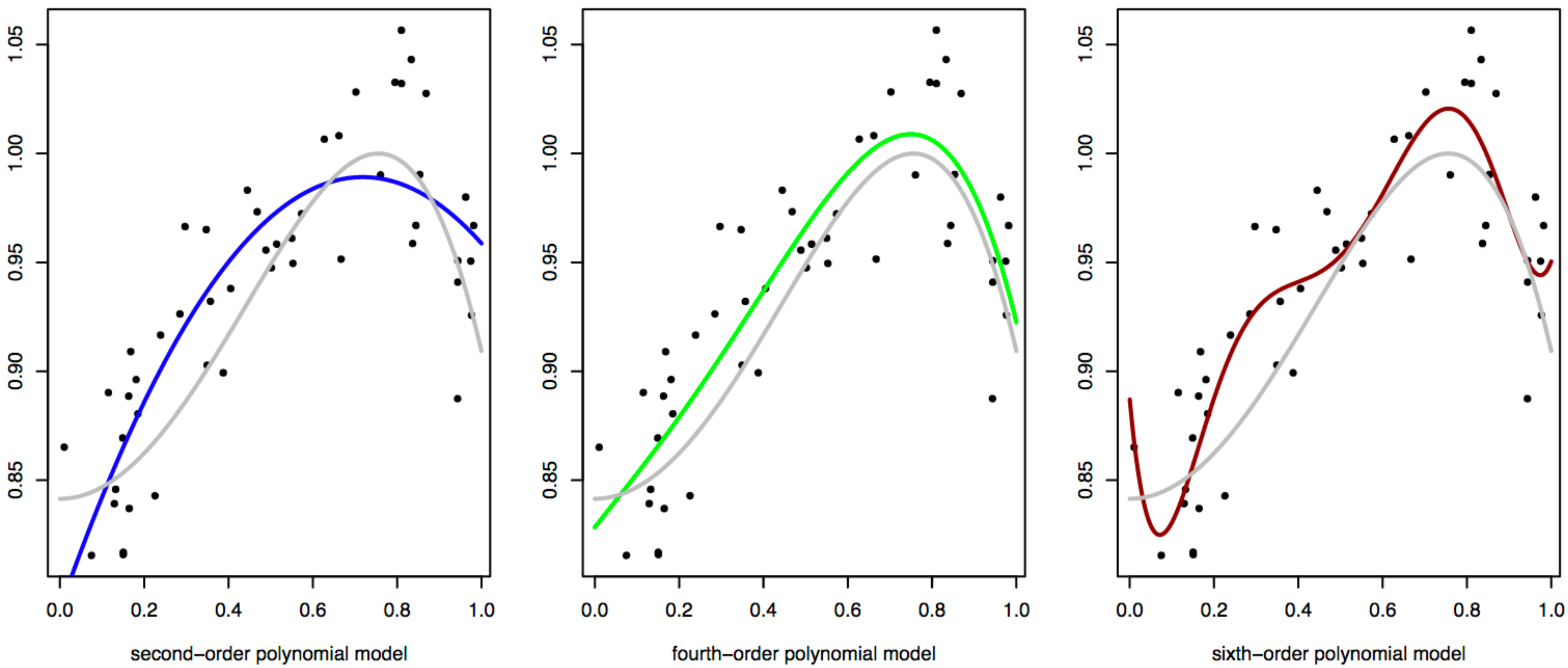
– Task: Learn $\mathbf{w}$ from training data $D = \{(x_i, t_i)\}$, $i = 1,..,N$

- Can be done by minimizing an error function that minimizes the misfit between $y(x,\mathbf{w})$ for any given $\mathbf{w}$ and training data
- One simple choice of error function is sum of squares of error between predictions $y(x_n,\mathrm{w})$ for each data point x_n and corresponding target values t_n so that we minimize

$$E(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{y(x_n,\mathrm{w}) - t_n\right\}^2$$

- It is zero when function $y(x,\mathrm{w})$ passes exactly through each training data point

Results with polynomial basis



Regression with multiple inputs

- Generalization
  - Predict value of continuous target variable t given value of D input variables $\mathrm{x}=[x_1,..x_D]$
  - t can also be a set of variables (multiple regression)
  - Linear functions of adjustable parameters
    - Specifically linear combinations of nonlinear functions of input variable
- Polynomial curve fitting is good only for:
  - Single input variable scalar x
  - It cannot be easily generalized to several variables, as we will see

Simplest Linear Model with D inputs

- Regression with D input variables

$$y(\mathrm{x},\mathrm{w}) = w_0 + w_1 x_1 + .. + w_d\, x_D = \mathrm{w}^T\mathrm{x}$$

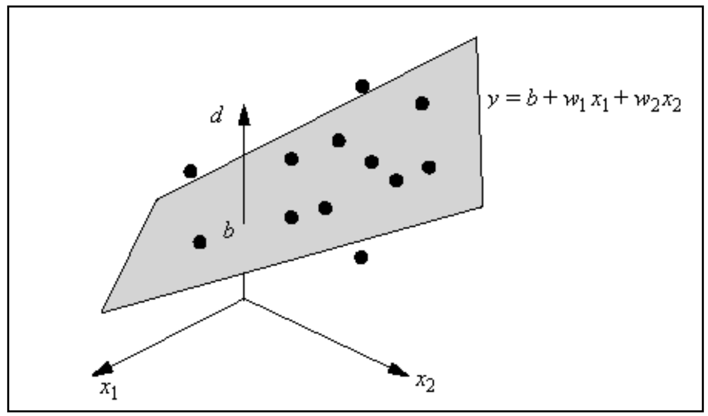
This differs from
Linear Regression with one variable
and Polynomial Reg with one variable

where $\mathrm{x}=(x_1,..,x_D)^{\mathrm{T}}$ are the input variables

- Called Linear Regression since it is a linear function of
  - parameters $w_0,..,w_D$
  - input variables $x_1,..,x_D$
- Significant limitation since it is a linear function of input variables
  - In the one-dimensional case this amounts a straight-line fit (degree-one polynomial)
  - $y(x,\mathrm{w}) = w_0 + w_1 x$

Fitting a Regression Plane

- Assume t is a function of inputs $x_1,\ x_2, \ldots x_D$
  Goal: find best linear regressor of t on all inputs
  - Fitting a hyperplane through N input samples
  - For $D = 2$:



x_1	x_2	t
1	2	2
2	5	1
2	3	2
2	2	2
3	4	1
3	5	3
4	6	2
5	5	3
5	6	4
5	7	3
6	8	4
7	6	2
8	4	4
8	9	3
9	8	4

- Being a linear function of input variables imposes limitations on the model
  - Can extend class of models by considering fixed nonlinear functions of input variables

Basis Functions

- In many applications, we apply some form of fixed-preprocessing, or feature extraction, to the original data variables
- If the original variables comprise the vector $\mathbf{x}$, then the features can be expressed in terms of basis functions $\{\phi_j(\mathbf{x})\}$
  - By using nonlinear basis functions we allow the function $y(\mathbf{x},\mathbf{w})$ to be a nonlinear function of the input vector $\mathbf{x}$
    - They are linear functions of parameters (gives them simple analytical properties), yet are nonlinear wrt input variables

Linear Regression with M Basis Functions

- Extended by considering nonlinear functions of input variables

$$y(\mathrm{x},\mathrm{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathrm{x})$$

  - where $\phi_j(\mathrm{x})$ are called Basis functions
  - We now need M weights for basis functions instead of D weights for features
  - With a dummy basis function $\phi_0(\mathrm{x})=1$ corresponding to the bias parameter w_0, we can write

$$y(\mathrm{x},\mathrm{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathrm{x}) = \mathrm{w}^T \phi(\mathrm{x})$$

  - where $\mathrm{w}=(w_0,w_1,..,w_{M-1})$ and $\Phi=(\phi_0,\phi_1,..,\phi_{M-1})^{\mathrm{T}}$

- Basis functions allow non-linearity with D input variables

Choice of Basis Functions

- Many possible choices for basis function:
  1. Polynomial regression
     - Good only if there is only one input variable
  2. Gaussian basis functions
  3. Sigmoidal basis functions
  4. Fourier basis functions
  5. Wavelets

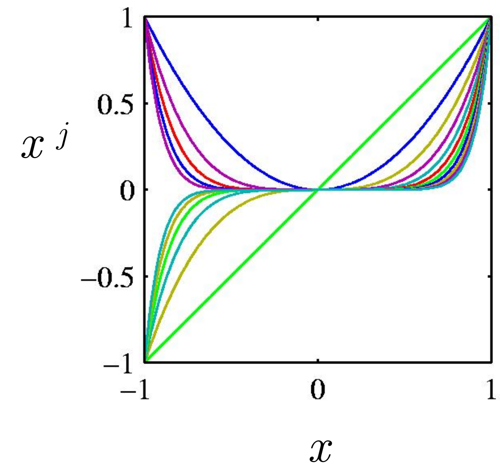
1. Polynomial Basis for one variable

- Linear Basis Function Model

$$y(x,\mathrm{w}) = \sum_{j=0}^{M-1} w_j \phi_j(x) = \mathrm{w}^T \phi(x)$$

- Polynomial Basis (for single variable x)

  $\phi_j(x) = x^j$ with degree M-1 polynomial



- Disadvantage
  - Global:
    - changes in one region of input space affects others
  - Difficult to formulate
    - Number of polynomials increases exponentially with M
  - Can divide input space into regions
    - use different polynomials in each region:
    - equivalent to spline functions

Can we use Polynomial with D variables? (Not practical!)

- Consider (for a vector x) the basis: $\phi_j(\mathrm{x}) = \|\mathrm{x}\|^j = \left[\sqrt{x_1^2 + x_2^2 + .. + x_d^2}\right]^j$
  - $\mathrm{x}=(2,1)$ and $\mathrm{x}=(1,2)$ have the same squared sum, so it is unsatisfactory
  - Vector is being converted into a scalar value thereby losing information
- Better polynomial approach:
  - Polynomial of degree M-1 has terms with variables taken none, one, two… M-1 at a time.
  - Use multi-index $j=(j_1,j_2,..j_D)$ such that $j_1+j_2+..j_D \leq M$-1
  - For a quadratic (M=3) with three variables (D=3)

$$y(\mathrm{x},\mathrm{w}) = \sum_{(j_1,j_2,j_3)} w_j \phi_j(\mathrm{x}) = w_0 + w_{1,0,0}x_1 + w_{0,1,0}x_2 + w_{0,0,1}x_3 + w_{1,1,0}x_1x_2 + w_{1,0,1}x_1x_3 + w_{0,1,1}x_2x_3 + w_{2,0,0}x_1^2 + w_{0,2,0}x_2^2 + w_{0,0,2}x_3^2$$

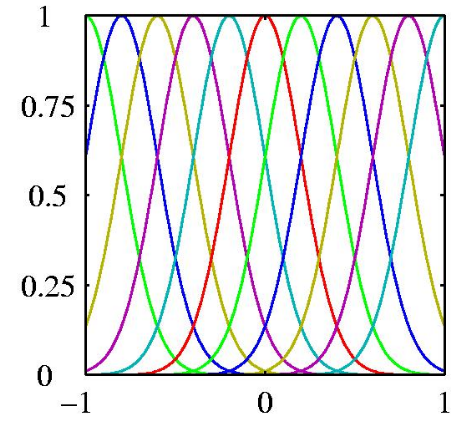
  - Number of quadratic terms is $1+D+D(D\text{-}1)/2+D$
  - For D=46, it is 1128
- Better to use Gaussian kernel, discussed next

Disadvantage of Polynomial

- Polynomials are *global* basis functions
  - Each affecting the prediction over the whole input space
- Often local basis functions are more appropriate

2. Gaussian Radial Basis Functions

- Gaussian $$\phi_j(x) = \exp\left(\frac{(x-\mu_j)^2}{2\sigma^2}\right)$$
  - Does not necessarily have a probabilistic interpretation
  - Usual normalization term is unimportant
    - since basis function is multiplied by weight w_j



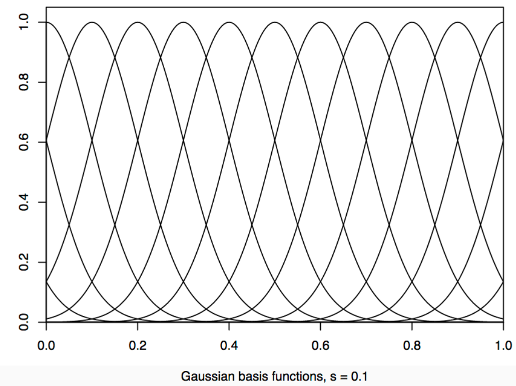
- Choice of parameters
  - μ_j govern the locations of the basis functions
    - Can be an arbitrary set of points within the range of the data
      - Can choose some representative data points
  - σ governs the spatial scale
    - Could be chosen from the data set e.g., average variance
- Several variables
  - A Gaussian kernel would be chosen for each dimension
  - For each j a different set of means would be needed– perhaps chosen from the data

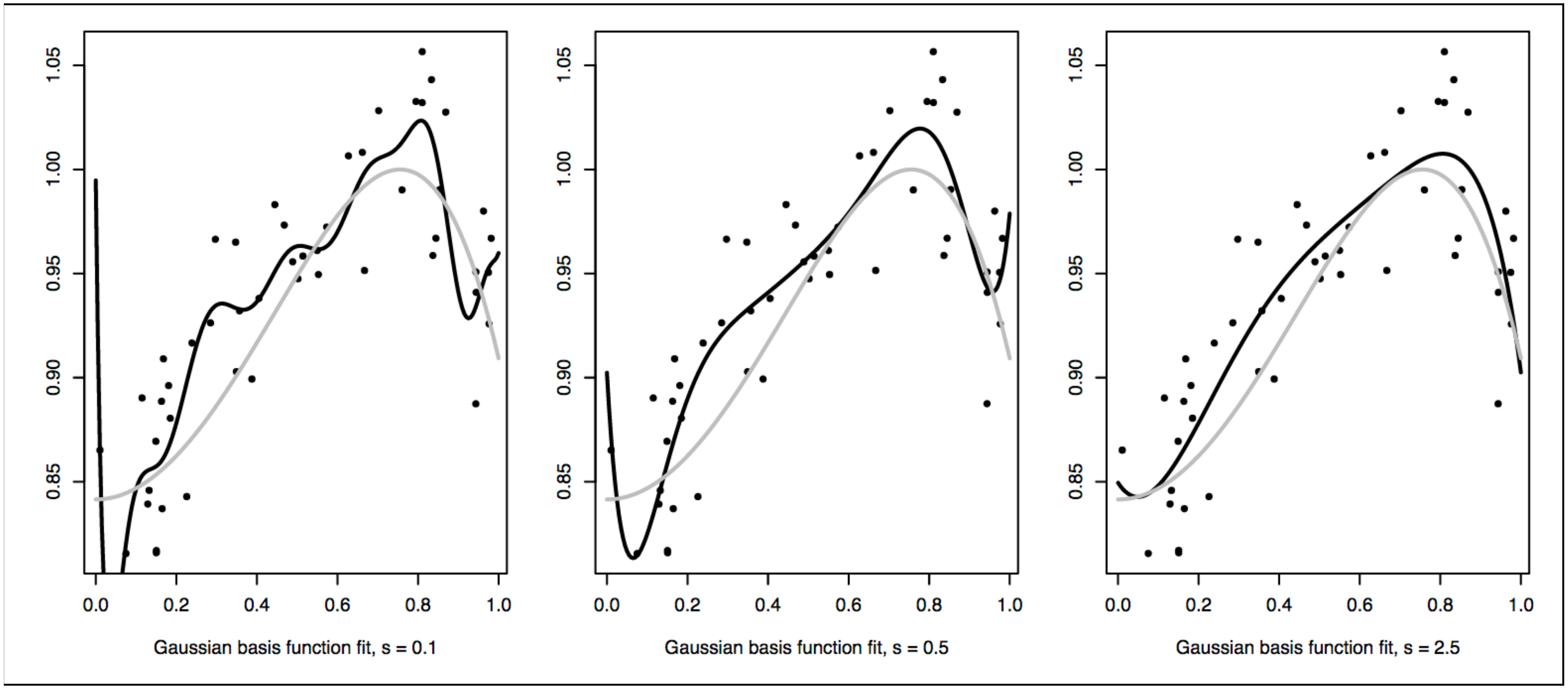
$$\phi_j(\mathrm{x}) = \exp\left(-\frac{1}{2}(\mathrm{x}-\boldsymbol{\mu}_j)^t \Sigma^{-1}(\mathrm{x}-\boldsymbol{\mu}_j)\right)$$

Result with Gaussian Basis Functions

$$\phi_j(x) = \exp(-(x-\mu_j)^2/2s^2)$$

Basis functions for $s=0.1$, with the μ_j on a grid with spacing s



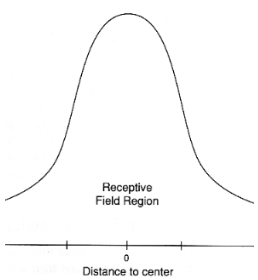


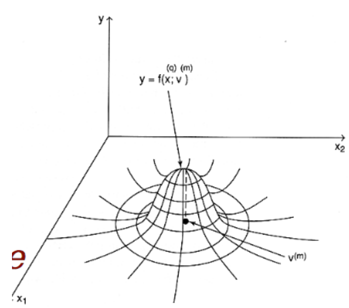
w_j s for middle model:

6856.5
-3544.1
-2473.7
-2859.8
-2637.7
-2861.5
-2468.0
-3558.4

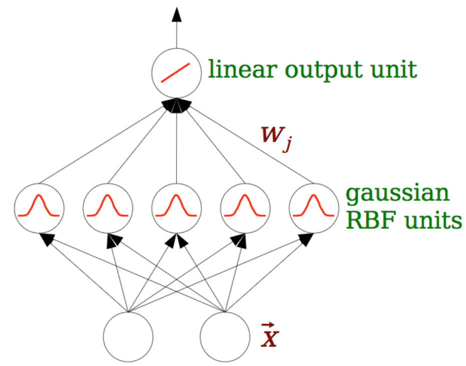
Biological Inspiration for RBFs

- Nervous system contains many examples
  - Local receptive fields in visual cortex





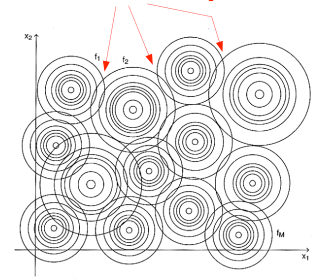
- RBF Network



$$\boxed{Output = \sum_j w_j \cdot \exp\left(\frac{-\|\vec{x}-\vec{\mu}_j\|^2}{\sigma_j^2}\right)}$$

- Receptive fields overlap
- So there is usually more than one unit active
- But for given input, total no. of active units is small

Tiling the input space



- Determining centers
  - k-means clustering
    - Choose k cluster centers
    - Mark each training point as captured by cluster to which it is closest
    - Move each cluster center to mean of points it captured
- Determining variance σ^2

  Global: σ =mean distance between each unit j and its closest neighbor

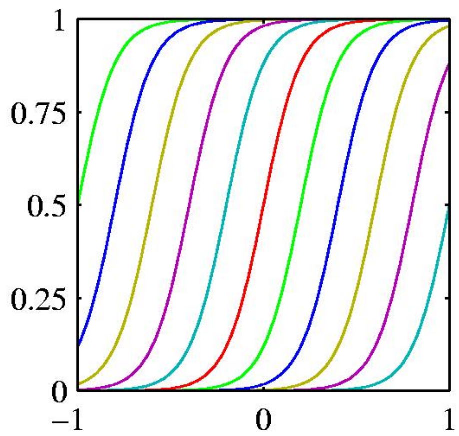
  P-nearest neighbor: set each σ_j so that there is certain overlap with P closest neighbors of unit j

3. Sigmoidal Basis Function

- Sigmoid $$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right) \quad \text{where} \quad \sigma(a) = \frac{1}{1+\exp(-a)}$$
- Equivalently, $\tanh$ because it is related to logistic sigmoid by

$$\tanh(a) = 2\sigma(a) - 1$$

Logistic Sigmoid
For different μ_j



4. Other Basis Functions

- Fourier
  - Expansion in sinusoidal functions
  - Infinite spatial extent
- Signal Processing
  - Functions localized in time and frequency
  - Called *wavelets*
    - Useful for lattices such as images and time series
- Further discussion independent of choice of basis including $\phi(\mathrm{x}) = \mathrm{x}$

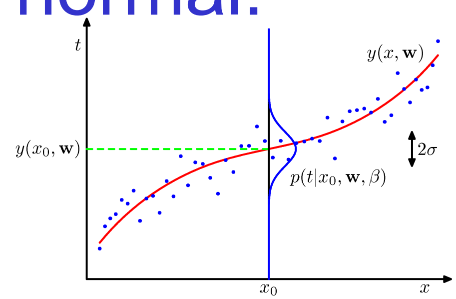
Relationship between Maximum Likelihood and Least Squares

- Will show that Minimizing sum-of-squared errors is the same as maximum likelihood solution under a Gaussian noise model
- Target variable is a scalar t given by deterministic function $y\,(\mathrm{x},\mathrm{w})$ with additive Gaussian noise ε

  $t = y(\mathrm{x},\mathrm{w}) + \varepsilon$

  – which is a *zero-mean* Gaussian with *precision* β
- Thus distribution of t is univariate normal:

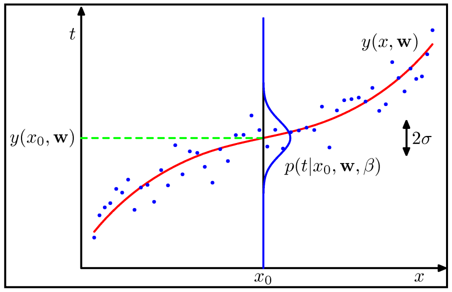
$$p(t|\mathrm{x},\mathrm{w},\beta) = N\,(t \mid \underbrace{y(\mathrm{x},\mathrm{w})}_{\text{mean}}, \underbrace{\beta^{-1}}_{\text{variance}})$$



Likelihood Function

- Data set:
  - Input $X=\{x_1,..x_N\}$ with target $\mathbf{t} = \{t_1,..t_N\}$
  - Target variables t_n are scalars forming a vector of size N
- Likelihood of the target data
  - It is the probability of observing the data assuming they are independent
  - since $p(t|\mathbf{x},\mathbf{w},\beta)=N(t \mid y(\mathbf{x},\mathbf{w}),\beta^{-1})$
  - and $y(\mathbf{x},\mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$

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



Log-Likelihood Function

- Likelihood

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

- Log-likelihood

$$\ln p(\mathrm{t} \mid \mathrm{w}, \beta) = \sum_{n=1}^{N} \ln N\left(t_n \mid \mathrm{w}^T \phi(\mathrm{x}_n), \beta^{-1}\right)$$

  – Using standard univariate Gaussian

$$N(x \mid \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

$$\ln p(\mathrm{t} \mid \mathrm{w}, \beta) = \frac{N}{2}\ln\beta - \frac{N}{2}\ln 2\pi - \beta E_D(\mathrm{w})$$

  - Where

$$E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{t_n - \mathrm{w}^T\phi(x_n)\right\}^2$$

Sum-of-squares Error Function

  - With Gaussian basis functions

$$\phi_j(\mathrm{x}) = \exp\left(\frac{(\mathrm{x}-\mu_j)^t(\mathrm{x}-\mu_j)}{2s^2}\right)$$

Maximizing Log-Likelihood Function

- Log-likelihood

$$\ln p(\mathrm{t} \mid \mathrm{w}, \beta) = \sum_{n=1}^{N} \ln N\left(t_n \mid \mathrm{w}^T \phi(\mathrm{x}_n), \beta^{-1}\right)$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln 2\pi - \beta E_D(\mathrm{w})$$

  - where

$$E_D(\mathrm{w}) = \frac{1}{2} \sum_{n=1}^{N} \left\{ t_n - \mathrm{w}^T \varphi(x_n) \right\}^2$$

- Therefore, maximizing likelihood is equivalent to minimizing $E_D(\mathrm{w})$

Determining max likelihood solution

- The likelihood function has the form

$$\ln p(\mathrm{t} \mid \mathrm{w}, \beta) = \frac{N}{2} \ln \beta - \frac{N}{2} \ln 2\pi - \beta E_D(\mathrm{w})$$

  - where

$$E_D(\mathrm{w}) = \frac{1}{2} \sum_{n=1}^{N} \left\{ t_n - \mathrm{w}^T \phi(\mathrm{x}_n) \right\}^2$$

- We will show that the maximum likelihood solution has a closed form

– Take derivative of $\ln p(\mathrm{t} \mid \mathrm{w}, \beta)$ wrt w and set equal to zero and solve for w

  – or equivalently just the derivative of $E_D(\mathrm{w})$

Gradient of Log-likelihood wrt w

$$\nabla \ln p(\mathrm{t} \mid \mathrm{w}, \beta) = \beta \sum_{n=1}^{N} \left\{ t_n - \mathrm{w}^T \phi(\mathrm{x}_n) \right\} \phi(\mathrm{x}_n)^T$$

-which is obtained from log-likelihood expression and by using calculus result

$$\nabla_w \left[-\frac{1}{2}\left(a - wb\right)^2\right] = (a - wb)b$$

- Gradient is set to zero and we solve for w

$$0 = \sum_{n=1}^{N} t_n \phi(\mathrm{x}_n) - \mathrm{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \phi(\mathrm{x}_n) \phi(\mathrm{x}_n)^T \right)$$

as shown in next slide

- Second derivative will be negative making this a maximum

Max Likelihood Solution for $\mathbf{w}$

- Solving for $\mathbf{w}$ we obtain:

$$\boxed{\mathbf{w}_{ML} = \Phi^{+}\mathbf{t}}$$

$X=\{\mathbf{x}_1,..\mathbf{x}_N\}$ are samples (vectors of d variables)
$\mathbf{t} = \{t_1,..t_N\}$ are targets (scalars)

where $\Phi^{+} = (\Phi^T\Phi)^{-1}\Phi^T$ is the Moore-Penrose pseudo inverse of the $N \times M$ Design Matrix Φ whose elements are given by $\Phi_{nj}=\phi_j(\mathbf{x}_n)$

- Known as the normal equations for the least squares problem

Design Matrix: Rows correspond to N samples, Columns to M basis functions

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \ldots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & & & \\ & & & \\ \phi_0(\mathbf{x}_N) & & & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

Pseudo inverse: generalization of notion of matrix inverse to non-square matrices
If design matrix is square and invertible. then pseudo-inverse is same as inverse

$\phi_i(\mathbf{x}_n)$ are M basis functions, e.g., Gaussians centered on M data points

$$\boxed{\phi_j(\mathbf{x}) = \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^t\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)\right)}$$

Design Matrix Φ

$\longleftarrow M$ Basis functions $\longrightarrow$

$$\Phi = \begin{pmatrix} \phi_0(\mathrm{x}_1) & \phi_1(\mathrm{x}_1) & \cdots & \phi_{M-1}(\mathrm{x}_1) \\ \phi_0(\mathrm{x}_2) & & & \\ & & & \\ \phi_0(\mathrm{x}_N) & & & \phi_{M-1}(\mathrm{x}_N) \end{pmatrix}$$

N Data

Represented as N-dim vectors

φ_0 φ_1 φ_{M-1}

Note that ϕ_0 corresponds to bias, which is set to 1

Φ is an $N \times M$ matrix

Thus Φ^T is an $M \times N$ matrix

Thus, $\Phi^T \Phi$ is $M \times M$, and so is $[\Phi^T \Phi]^{-1}$

So we have $[\Phi^T \Phi]^{-1} \times \Phi^T$ is $M \times N$

Since $\mathbf{t}$ is N x 1, we have that $\mathbf{w}_{ML} = [\Phi^T \Phi]^{-1} \times \Phi^T \mathrm{t}$ is $M \times 1$.

which consists of the M weights (including bias).

What is the role of Bias parameter w_0?

- Sum-of squares error function is: $E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathrm{w}^T\phi(\mathrm{x}_n)\}^2$
  - Substituting: $y(\mathrm{x},\mathrm{w}) = w_0 + \sum_{j=1}^{M-1} w_j\phi_j(\mathrm{x})$ we get:

$$E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{t_n - w_0 - \sum_{j=1}^{M-1} w_j\phi_j(\mathrm{x}_n)\right\}^2$$

  - Setting derivatives wrt w_0 equal to zero and solving for w_0

$$w_0 = \bar{t} - \sum_{j=1}^{M-1} w_j\overline{\phi_j}$$ where $$\bar{t} = \frac{1}{N}\sum_{n=1}^{N} t_n$$ and $$\bar{\phi}_j = \frac{1}{N}\sum_{n=1}^{N}\phi_j(\mathrm{x}_n)$$

    - First term is average of the N values of t
    - Second term is weighted sum of the average basis function values over N samples
- Thus bias w_0 compensates for difference between average target values and weighted sum of averages of basis function values

Maximum Likelihood for precision β

- We have determined m.l.e. solution for w using a probabilistic formulation
  - $p(t|\mathrm{x},\mathrm{w},\beta)=N(t|y(\mathrm{x},\mathrm{w}),\beta^{-1})$
  - With log-likelihood

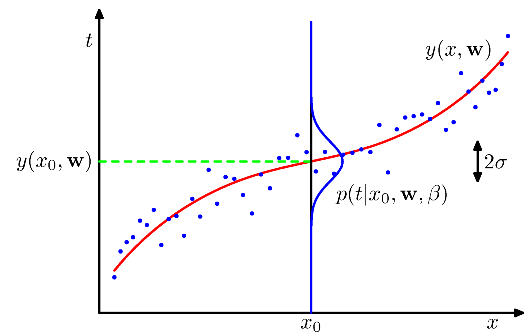
$$\boxed{\mathrm{w}_{ML} = \Phi^{+}\mathrm{t}}$$

$$\ln p(\mathrm{t}\,|\,\mathrm{w},\beta) = \frac{N}{2}\ln\beta - \frac{N}{2}\ln 2\pi - \beta E_D(\mathrm{w})$$

$$\nabla \ln p(\mathrm{t}\,|\,\mathrm{w},\beta) = \beta\sum_{n=1}^{N}\left\{\, t_n - \mathrm{w}^T\phi(\mathrm{x}_n)\,\right\}\phi(\mathrm{x}_n)^T$$

- Taking gradient wrt β gives

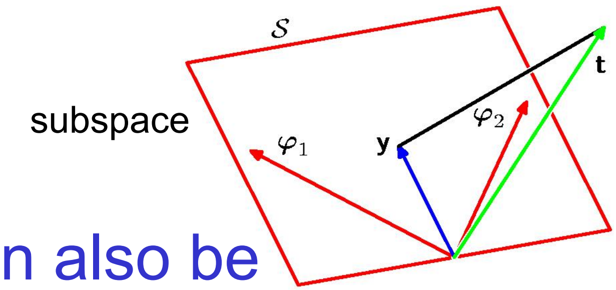
$$\boxed{\frac{1}{\beta_{ML}} = \frac{1}{N}\sum_{n=1}^{N}\left\{\, t_n - \mathrm{w}_{ML}^T\phi(\mathrm{x}_n)\,\right\}^2}$$



– Thus Inverse of the noise precision gives *Residual variance of the target values around the regression function*

Geometry of Least Squares

- Geometrical Interpretation of Least Squares Solution instructive
- Consider N-dim space with axes t_n
  so that $\mathrm{t} = (t_1,\ldots,t_\mathrm{N})^\mathrm{T}$ is a vector in this space



- Each basis $\boldsymbol{\phi}_j(\mathrm{x}_n)$ evaluated at N points can also be represented as a vector in the same space
- ϕ_j corresponds to j^{th} column of $\mathbf{\Phi}$, whereas $\phi(\mathrm{x_n})$ corresponds to the the n^{th} row of $\mathbf{\Phi}$
- If the no of basis functions is smaller than the no of data points
  - i.e., $M<N$ then the M vectors $\phi_j(\mathrm{x}_n)$ will span linear subspace S of dim M
- Define $\boldsymbol{y}$ to be an N-dim vector whose n^{th} element is $y(\mathrm{x}_n,\mathrm{w})$
- Sum-of-squares error is equal to squared Euclidean distance between $\boldsymbol{y}$ and t
- Solution w corresponds to $\boldsymbol{y}$ that lies in subspace S that is closest to t
  - Corresponds to orthogonal projection of t onto S

Difficulty of Direct solution

- Direct solution of normal equations

$$\boxed{\mathbf{w}_{ML} = \Phi^{+}\mathbf{t}} \qquad \boxed{\Phi^{+} = (\Phi^{T}\Phi)^{-1}\Phi^{T}}$$

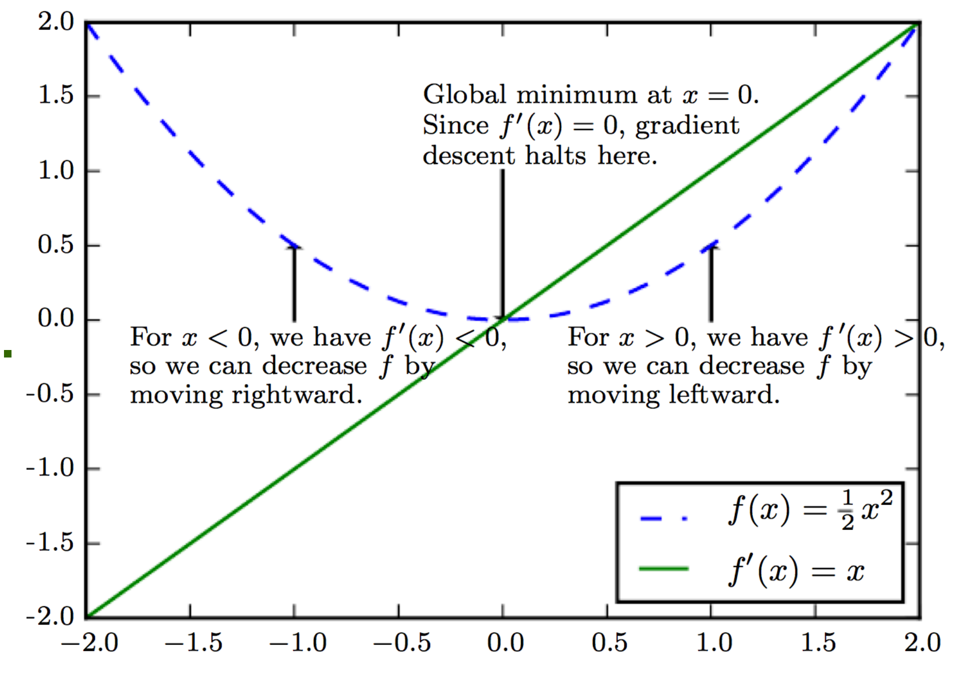
- This direct solution can lead to numerical difficulties
  - When $\Phi^T\Phi$ is close to singular (determinant=0)
  - When two basis functions are collinear parameters can have large magnitudes
- Not uncommon with real data sets
- Can be addressed using
  - Singular Value Decomposition
  - Addition of regularization term ensures matrix is non-singular

Method of Gradient Descent

- Criterion $f(x)$ minimized by moving from current solution in direction of negative of gradient $f'(x)$
- Steepest descent proposes a new point

$$\boxed{x' = x - \eta f'(x)}$$

  - where η is the learning
  - rate, a positive scalar.
  - Set to a small constant.



Gradient with multiple inputs

- For multiple inputs we need partial derivatives:

  $\boxed{\frac{\partial}{\partial x_i} f(\boldsymbol{x})}$ is how f changes as only x_i increases

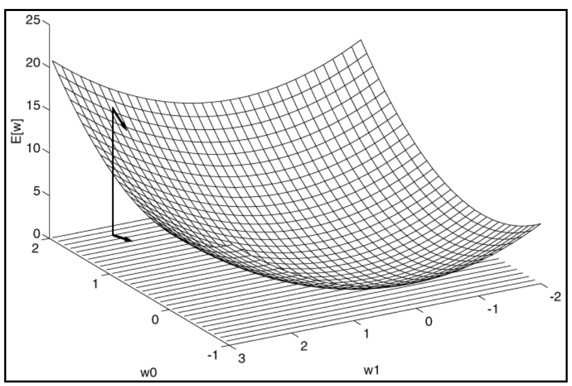
  – Gradient of f is a vector of partial derivatives $\boxed{\nabla_{\boldsymbol{x}} f\left(\boldsymbol{x}\right)}$

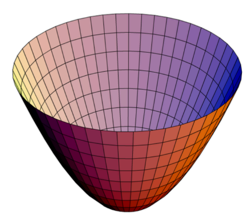
- Gradient descent proposes a new point

$$\boxed{\boldsymbol{x}' = \boldsymbol{x} - \eta \nabla_{\boldsymbol{x}} f\left(\boldsymbol{x}\right)}$$

  – where η is the learning rate, a positive scalar
    - Set to a small constant

Direction in w_0-w_1 plane producing steepest descent





Gradient Descent for Regression

- Error function $E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}^2$ sums over data
  - Denoting $E_D(\mathrm{w}) = \Sigma_n E_n$, update w using

$$\mathrm{w}^{(\tau+1)} = \mathrm{w}^{(\tau)} - \eta \nabla E_n$$

    - where τ is the iteration number and η is a learning rate parameter
- Substituting for the derivative $\nabla E_n = -\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}\phi(\mathrm{x}_n)^T$

$$\mathrm{w}^{(\tau+1)} = \mathrm{w}^{(\tau)} + \eta(t_n - \mathrm{w}^{(\tau)T}\phi_n)\phi_n$$

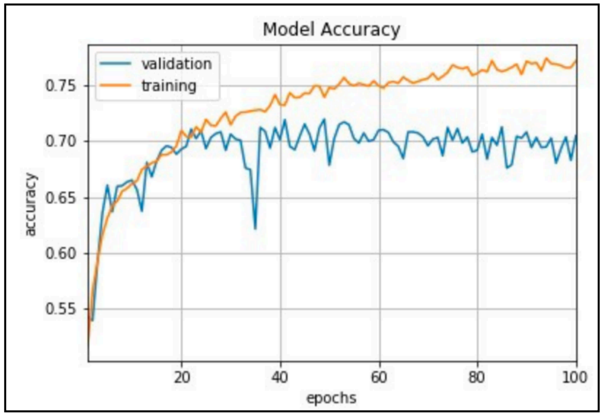
where $\phi_n = \phi(\mathrm{x}_n)$

    - w is initialized to some starting vector $\mathrm{w}^{(0)}$
    - η chosen with care to ensure convergence
- Known as *Least Mean Squares* Algorithm

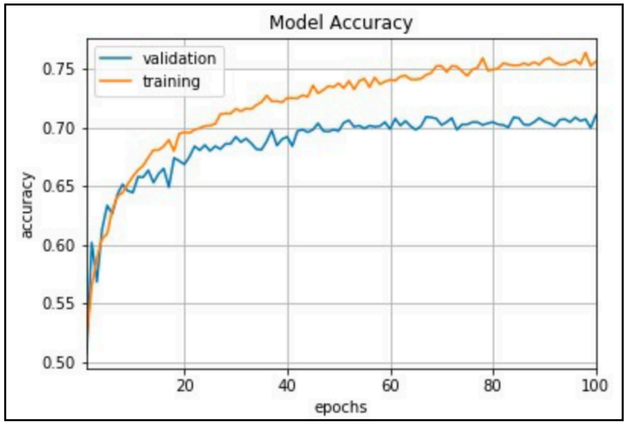
Choosing the Learning rate

- Useful to reduce η as training progresses
- Constant learning rate is default in Keras
  - Momentum and decay are set to 0 by default
    - keras.optimizers.SGD(lr=0.1, momentum=0.0, decay=0.0, nesterov=**False**)

Constant learning rate



Time-based decay: decay_rate=learning_rate/epochs)
SGD(lr=0.1, momentum=0.8, decay=decay_rate, Nesterov=False)



Sequential (On-line) Learning

- Maximum likelihood solution is

$$\mathrm{w}_{ML} = (\Phi^T \Phi)^{-1} \Phi^T \mathrm{t}$$

- It is a batch technique
  - Processing entire training set in one go
  - It is computationally expensive for large data sets
    - Due to huge N × M Design matrix Φ
- Solution: use a sequential algorithm where samples are presented one at a time (or a minibatch at a time)
  - Called *stochastic gradient descent*

Computational bottleneck

- A recurring problem in machine learning:
  - large training sets are necessary for good generalization
  - but large training sets are also computationally expensive
- SGD is an extension of gradient descent that offers a solution
  - Moreover it is a method of generalization beyond the training set

Insight of SGD

- Gradient is an expectation $\nabla \ln p(y \mid X, \theta, \beta) = \beta \sum_{i=1}^{m} \left\{ y^{(i)} - \theta^T \boldsymbol{x}^{(i)} \right\} \boldsymbol{x}^{(i)T}$
  - Expectation may be approximated using small set of samples
- In each step of SGD we can sample a *minibatch* of examples $B = \{x^{(1)}, \ldots, x^{(m')}\}$
  - drawn uniformly from the training set
  - Minibatch size m' is typically chosen to be small: 1 to a hundred
    - Crucially m' is held fixed even if sample set is in billions
    - We may fit a training set with billions of examples using updates computed on only a hundred examples

Regularized Least Squares

- As model complexity increases, e.g., degree of polynomial or no.of basis functions, then it is likely that we overfit
- One way to control overfitting is not to limit complexity but to add a regularization term to the error function
- Error function to minimize takes the form

$$E(\mathrm{w}) = E_D(\mathrm{w}) + \lambda E_W(\mathrm{w})$$

  - where λ is the *regularization coefficient* that controls relative importance of data-dependent error $E_D(\mathrm{w})$ and regularization term $E_W(\mathrm{w})$

Simplest Regularizer is weight decay

- Regularized least squares is

$$\boxed{E(\mathrm{w}) = E_D(\mathrm{w}) + \lambda E_W(\mathrm{w})}$$

- Simple form of regularization term is

$$\boxed{E_W(\mathrm{w}) = \frac{1}{2}\mathrm{w}^T\mathrm{w}}$$

  – Thus total error function becomes

$$\boxed{E(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(x_n) \right\}^2 + \frac{\lambda}{2}\mathrm{w}^T\mathrm{w}}$$

- This regularizer is called *weight decay*
  – because in sequential learning weight values decay towards zero unless supported by data
- Also, the error function remains a *quadratic function* of w, so exact minimizer found in closed form

Closed-form Solution with Regularizer

- Error function with *quadratic regularizer is*,

$$\boxed{E(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{\ t_n - \mathrm{w}^T\phi(x_n)\ \right\}^2 + \frac{\lambda}{2}\mathrm{w}^T\mathrm{w}}$$

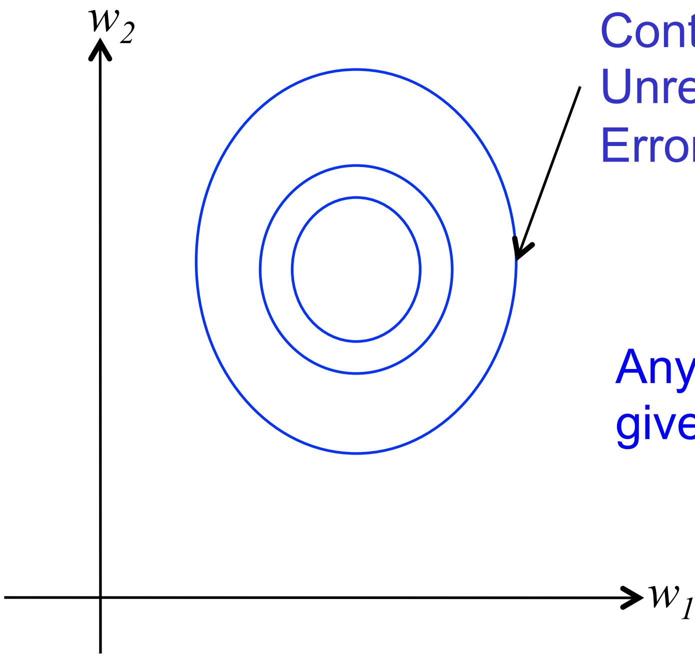
- Its exact minimizer can be found in closed form
  - By setting gradient wrt w to zero and solving for w

$$\boxed{\mathrm{w} = (\lambda \mathrm{I} + \Phi^T\Phi)^{-1}\Phi^T\mathrm{t}}$$

- This is a simple extension of the least squared solution

$$\boxed{\mathrm{w}_{ML} = (\Phi^T\Phi)^{-1}\Phi^T\mathrm{t}}$$

Geometric Interpretation of Regularizer



Contours of Unregularized Error function

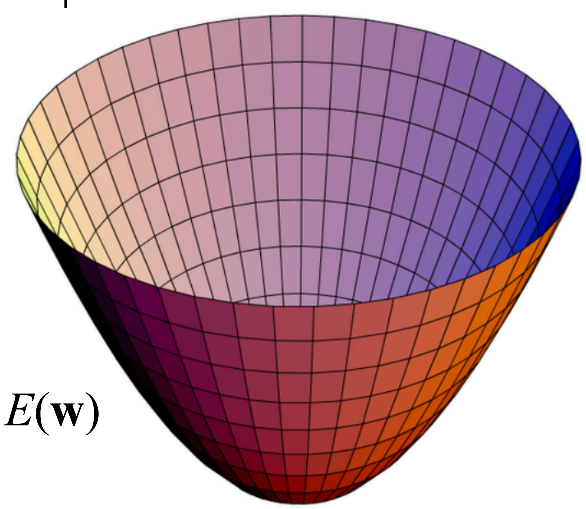
In *unregularized* case:
we are trying to find w that minimizes

$$\boxed{E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}^2}$$

Any value of w on contour gives same error

In *regularized* case:
choose that value of w subject to the constraint

$$\boxed{\sum_{j=1}^{M} | w_j |^2 \leq \eta}$$



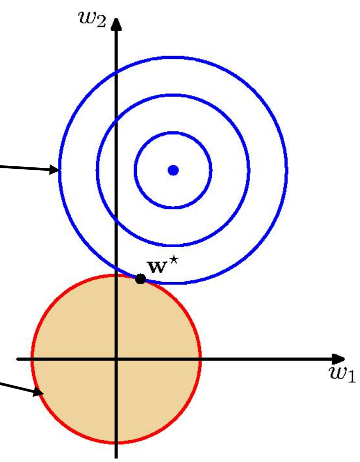
$E(\mathbf{w})$

We don't want the weights to become too large
The two approaches related by Lagrange multipliers

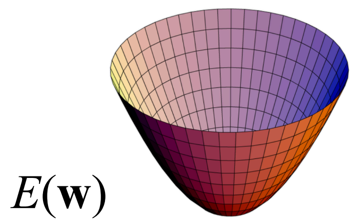
$$\boxed{E(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(x_n) \right\}^2 + \frac{\lambda}{2}\mathrm{w}^T\mathrm{w}}$$

Minimization of Unregularized Error subject to constraint

- Blue: Contours of unregularized error function
- Constraint region
- w^* is optimum value



Minimization With quadratic Regularizer, $q=2$



A more general regularizer

- Regularized Error

$$\frac{1}{2}\sum_{n=1}^{N}\{\ t_n - \mathrm{w}^T\phi(\mathrm{x}_n)\ \}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|\ w_j\ |^q$$

- Where $q=2$ corresponds to the *quadratic* regularizer

  $q=1$ is known as *lasso*

- Lasso has the property that if λ is sufficiently large some of the coefficients w_j are driven to zero leading to a sparse model in which the corresponding basis functions play no role

Contours of regularization term

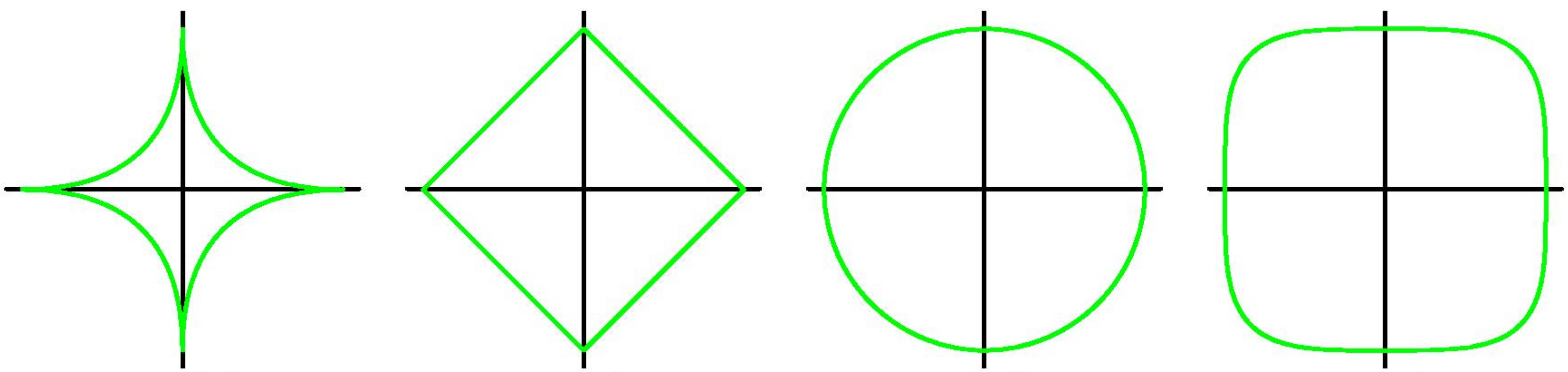
$$\frac{1}{2}\sum_{n=1}^{N}\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}| w_j |^q$$

- Contours of regularization term $|w_j|^q$ for values of q

Space of w_1,w_2

Any choice along the contour has the same value of w

$\sqrt{w_1} + \sqrt{w_2} = const$ $\quad w_1 + w_2 = const$ $\quad w_1^{\ 2} + w_2^{\ 2} = const$ $\quad w_1^{\ 4} + w_2^{\ 4} = const$



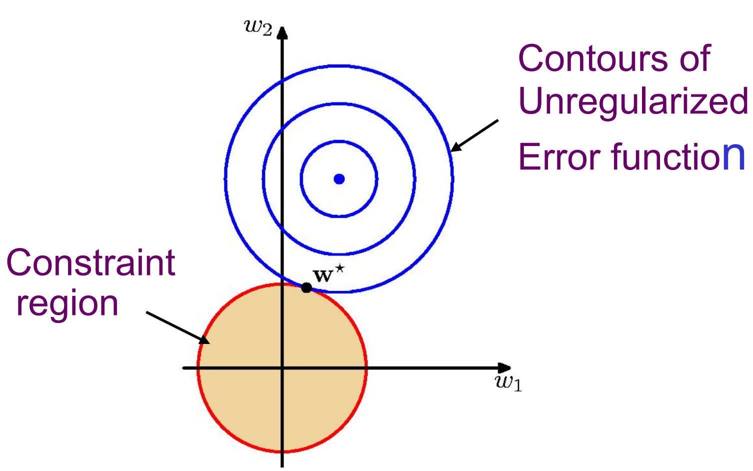
$q = 0.5$ $\quad q = 1$ $\quad q = 2$ $\quad q = 4$

Lasso Quadratic

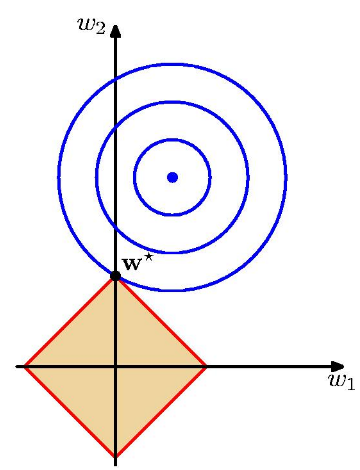
Sparsity with Lasso constraint

- With q=1 and λ is sufficiently large, some of the coefficients w_j are driven to zero
- Leads to a sparse model
  - where corresponding basis functions play no role
- Origin of sparsity is illustrated here:

Quadratic solution where w_1* and w_0* are nonzero



Minimization with Lasso Regularizer
A sparse solution with w_1*=0



Regularization: Conclusion

- Regularization allows
  - complex models to be trained on small data sets
  - without severe over-fitting
- It limits model complexity
  - i.e., how many basis functions to use?
- Problem of limiting complexity is shifted to
  - one of determining suitable value of regularization coefficient

Linear Regression Summary

- Linear Regression with M basis functions:

$$\boxed{y(\mathrm{x},\mathrm{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathrm{x}) = \mathrm{w}^T\phi(\mathrm{x})}$$

$$\boxed{\phi_j(\mathrm{x}) = \exp\left(-\frac{1}{2}(\mathrm{x}-\boldsymbol{\mu}_j)^t \Sigma^{-1}(\mathrm{x}-\boldsymbol{\mu}_j)\right)}$$

- Objective Function *without/with* regularization is

$$\boxed{E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}^2}$$

$$\boxed{E_D(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(x_n) \right\}^2 + \frac{\lambda}{2}\mathrm{w}^T\mathrm{w}}$$

- Closed-form ML solution is:

$$\boxed{\mathrm{w}_{ML} = (\Phi^T\Phi)^{-1}\Phi^T\mathrm{t}}$$

$$\boxed{\mathrm{w}_{ML} = (\lambda I + \Phi^T\Phi)^{-1}\Phi^T\mathrm{t}}$$

$$\boxed{\Phi = \begin{pmatrix} \phi_0(\mathrm{x}_1) & \phi_1(\mathrm{x}_1) & \ldots & \phi_{M-1}(\mathrm{x}_1) \\ \phi_0(\mathrm{x}_2) & & & \\ & & & \\ \phi_0(\mathrm{x}_N) & & & \phi_{M-1}(\mathrm{x}_N) \end{pmatrix}}$$

- Gradient Descent: $\mathrm{w}^{(\tau+1)} = \mathrm{w}^{(\tau)} - \eta\nabla E_n$

$$\boxed{\nabla E_n = -\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}\phi(\mathrm{x}_n)^T}$$

$$\boxed{\nabla E_n = \left[-\sum_{n=1}^{N}\left\{ t_n - \mathrm{w}^T\phi(\mathrm{x}_n) \right\}\phi(\mathrm{x}_n)^T\right] + \lambda\mathrm{w}}$$

Returning to LeToR Problem

- Try:
- Several Basis Functions
- Quadratic Regularization
- Express results as E_{RMS}
  - rather than as squared error $E(\mathbf{w}^*)$ or as Error Rate with thresholded results

$$E_{RMS} = \sqrt{2E(\mathbf{w}^*)/N}$$

Multiple Outputs

- Several target variables $\mathbf{t} = (t_1,..,t_K) \quad K > 1$
- Can be treated as multiple (K) independent regression problems
  - Different basis functions for each component of $\mathbf{t}$
- More common solution: same set of basis functions to model all components of target vector $\mathbf{y}(\mathbf{x},\mathbf{w}) = \mathbf{W}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$
  - where $\mathbf{y}$ is a K-dim column vector, $\mathbf{W}$ is a M x K matrix of weights and $\phi(\mathbf{x})$ is a M-dimensional column vector with with elements $\phi_j(\mathbf{x})$

Solution for Multiple Outputs

- Set of observations $\mathbf{t}_1,..,\mathbf{t}_N$ are combined into a matrix T of size N x K such that the n^{th} row is given by $\mathrm{t}_n{}^{\mathrm{T}}$
- Combine input vectors $\mathrm{x}_1,..,\mathrm{x}_N$ into matrix X
- Log-likelihood function is maximized

- Solution is similar: $\mathrm{W}_{\mathrm{ML}}=(\Phi^{\mathrm{T}}\Phi)^{-1}\Phi^{\mathrm{T}}\mathrm{T}$