Advanced Machine Learning
Summer 2019

Part 3 – Linear Regression II
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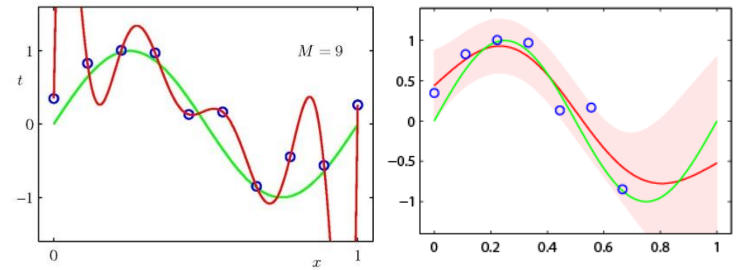
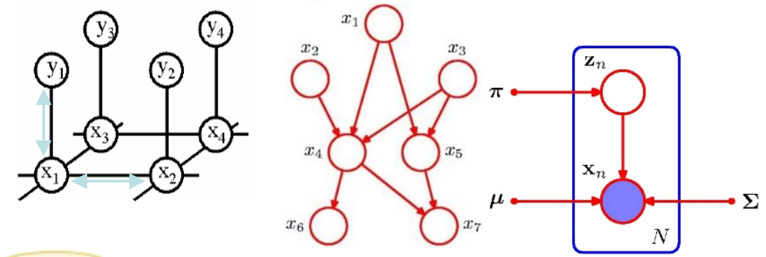
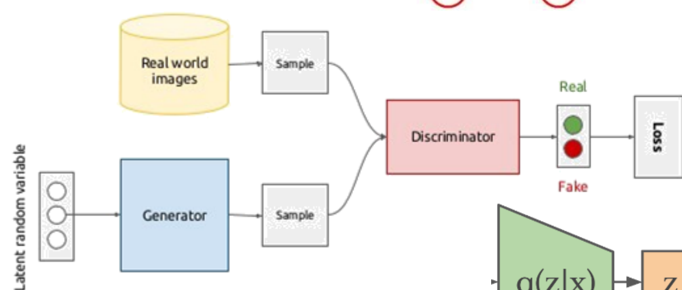
Course Outline

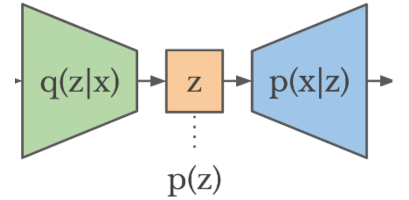
- Regression Techniques
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Bayesian Regression
- Deep Reinforcement Learning
- Probabilistic Graphical Models
  - Bayesian Networks
  - Markov Random Fields
  - Inference (exact & approximate)
- Deep Generative Models
  - Generative Adversarial Networks
  - Variational Autoencoders

$$f : \mathcal{X} \rightarrow \mathbb{R}$$









Topics of This Lecture

- Recap: Probabilistic View on Regression
- Properties of Linear Regression
  - Loss functions for regression
  - Basis functions
  - Multiple Outputs
- Regularization revisited
  - Regularized Least-squares
  - The Lasso
  - Discussion

Recap: Probabilistic Regression

- First assumption:
  - Our target function values y are generated by adding noise to the function estimate:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon$$

Target function value

Regression function

Input value

Weights or parameters

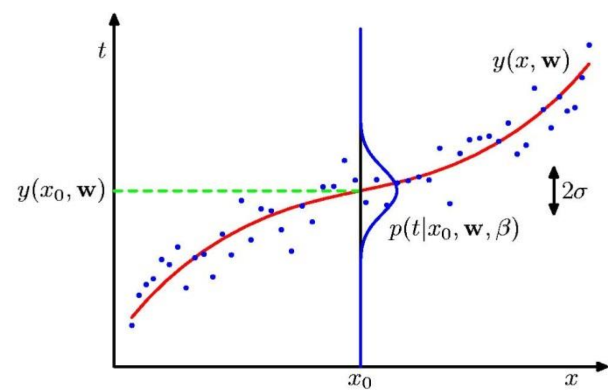
Noise

- Second assumption:
  - The noise is Gaussian distributed

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

Mean

Variance (β precision)



Slide credit: Bernt Schiele

Recap: Probabilistic Regression

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{t} = [t_1, \dots, t_n]^T$

- Conditional likelihood (assuming i.i.d. data)

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n | y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}) = \prod_{n=1}^{N} \mathcal{N}(t_n | \underbrace{\mathbf{w}^T \phi(\mathbf{x}_n)}_{\text{Generalized linear regression function}}, \beta^{-1})$$

$\Rightarrow$ Maximize w.r.t. $\mathbf{w}$, β

Slide credit: Bernt Schiele

Recap: Maximum Likelihood Regression

$$\nabla_{\mathbf{w}} \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) \;=\; -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n))\phi(\mathbf{x}_n)$$

- Setting the gradient to zero:

$$\begin{aligned}
0 \;&=\; -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n))\phi(\mathbf{x}_n) \\
\Leftrightarrow\; \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n) &= \left[\sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T\right] \mathbf{w} \\
\Leftrightarrow\; \boldsymbol{\Phi}\mathbf{t} &= \boldsymbol{\Phi}\boldsymbol{\Phi}^T \mathbf{w} \qquad\qquad \boldsymbol{\Phi} = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)] \\
\Leftrightarrow\; \mathbf{w}_{\mathrm{ML}} &= (\boldsymbol{\Phi}\boldsymbol{\Phi}^T)^{-1}\boldsymbol{\Phi}\mathbf{t}
\end{aligned}$$

Same as in least-squares regression!

$\Rightarrow$ *Least-squares regression is equivalent to Maximum Likelihood under the assumption of Gaussian noise.*

Slide credit: Bernt Schiele

Recap: Role of the Precision Parameter

- Also use ML to determine the precision parameter β:

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\log\beta - \frac{N}{2}\log(2\pi)$$

- Gradient w.r.t. β:

$$\nabla_\beta \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \frac{N}{2}\frac{1}{\beta}$$

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

$\Rightarrow$ *The inverse of the noise precision is given by the residual variance of the target values around the regression function.*

Recap: Predictive Distribution

- Having determined the parameters $\mathbf{w}$ and β, we can now make predictions for new values of $\mathbf{x}$.

$$p(t|\mathbf{X}, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1})$$

- This means
  - Rather than giving a point estimate, we can now also give an estimate of the estimation uncertainty.

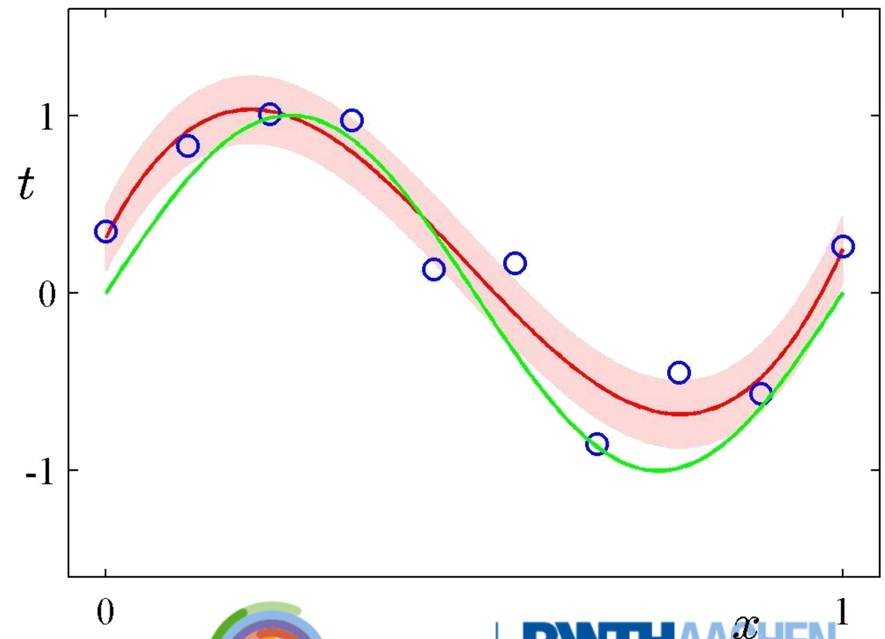


Image source: C.M. Bishop, 2006

Recap: Maximum-A-Posteriori Estimation

- Introduce a prior distribution over the coefficients $\mathbf{w}$.
  - For simplicity, assume a zero-mean Gaussian distribution

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

  - New hyperparameter α controls the distribution of model parameters.

- Express the posterior distribution over $\mathbf{w}$.
  - Using Bayes' theorem:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

  - We can now determine $\mathbf{w}$ by maximizing the posterior.
  - This technique is called maximum-a-posteriori (MAP).

Recap: MAP Solution

- Minimize the negative logarithm

$$-\log p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) \propto \underline{-\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)} \underline{- \log p(\mathbf{w}|\alpha)}$$

$$\underline{-\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta)} = \frac{\beta}{2} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2 + \text{const}$$

$$\underline{-\log p(\mathbf{w}|\alpha)} = \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \text{const}$$

- The MAP solution is therefore the solution of

$$\frac{\beta}{2} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2 + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w}$$

$\Rightarrow$ *Maximizing the posterior distribution is equivalent to minimizing the regularized sum-of-squares error (with* $\lambda = \frac{\alpha}{\beta}$*).*

MAP Solution (2)

$$\nabla_{\mathbf{w}} \log p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \beta, \alpha) = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n))\phi(\mathbf{x}_n) + \alpha \mathbf{w}$$

- Setting the gradient to zero:

$$0 = -\beta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \phi(\mathbf{x}_n))\phi(\mathbf{x}_n) + \alpha \mathbf{w}$$

$$\Leftrightarrow \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n) = \left[\sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T\right] \mathbf{w} + \frac{\alpha}{\beta}\mathbf{w}$$

$$\Leftrightarrow \boldsymbol{\Phi}\mathbf{t} = \left(\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \frac{\alpha}{\beta}\mathbf{I}\right)\mathbf{w} \qquad \boldsymbol{\Phi} = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]$$

$$\Leftrightarrow \mathbf{w}_{\mathrm{MAP}} = \left(\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \frac{\alpha}{\beta}\mathbf{I}\right)^{-1} \boldsymbol{\Phi}\mathbf{t}$$

Effect of regularization: Keeps the inverse well-conditioned

Recap: Bayesian Curve Fitting

- Given
  - Training data points: $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
  - Associated function values: $\mathbf{t} = [t_1, \ldots, t_n]^T$
  - Our goal is to predict the value of t for a new point $\mathbf{x}$.

- Evaluate the predictive distribution

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

What we just computed for MAP

  - Noise distribution – again assume a Gaussian here

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

  - Assume that parameters α and β are fixed and known for now.

Bayesian Curve Fitting

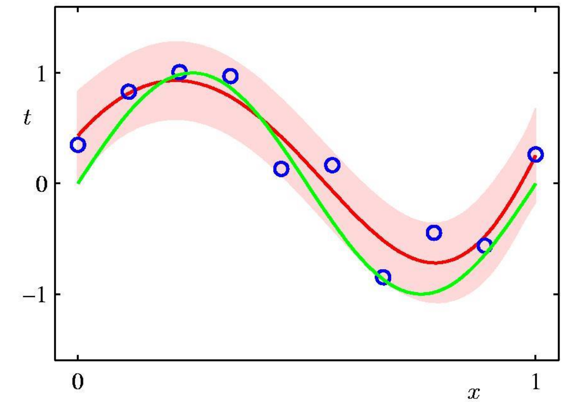
- Under those assumptions, the posterior distribution is a Gaussian and can be evaluated analytically:

$$p(t|x, \mathbf{X}, \mathbf{t}) = \mathcal{N}(t|m(x), s^2(x))$$

  – where the mean and variance are given by

$$m(x) = \beta\phi(x)^T\mathbf{S}\sum_{n=1}^{N}\phi(\mathbf{x}_n)t_n$$

$$s(x)^2 = \beta^{-1} + \phi(x)^T\mathbf{S}\phi(x)$$



  – and $\mathbf{S}$ is the regularized covariance matrix

$$\mathbf{S}^{-1} = \alpha\mathbf{I} + \beta\sum_{n=1}^{N}\phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T$$

Image source: C.M. Bishop, 2006

Analyzing the result

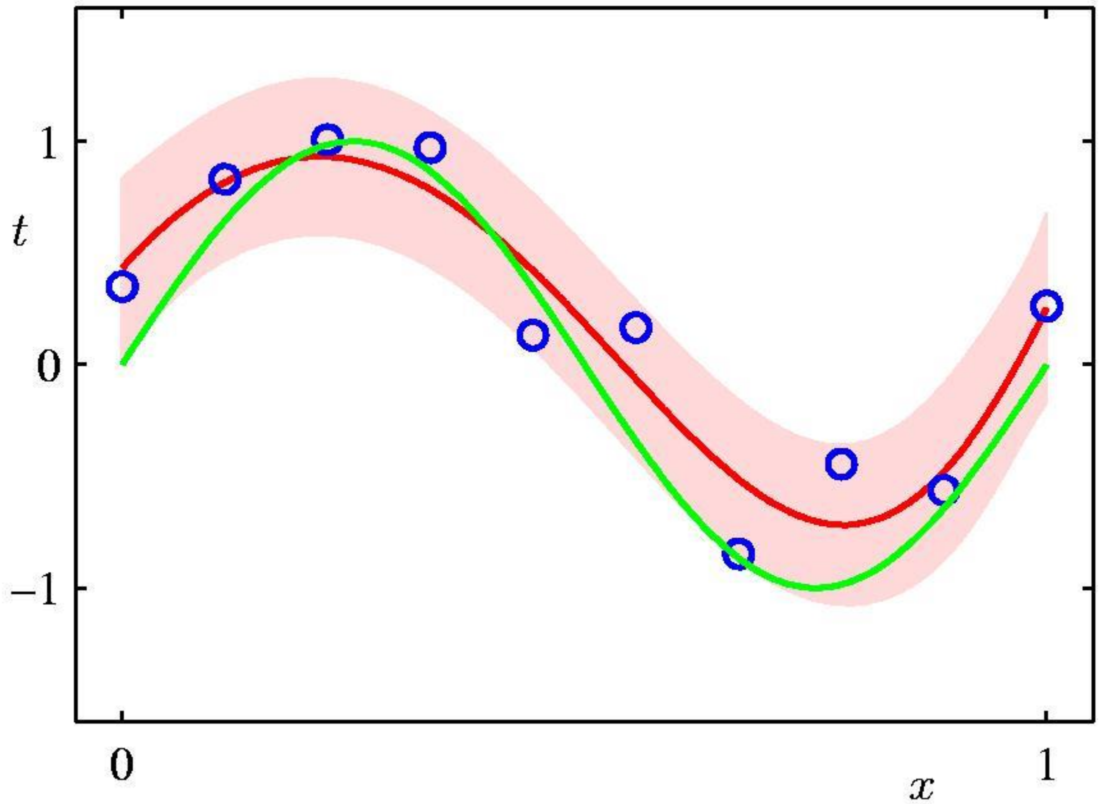
- Analyzing the variance of the predictive distribution

$$s(x)^2 = \underbrace{\beta^{-1}}_{} + \underbrace{\phi(x)^T \mathbf{S} \phi(x)}_{}$$

Uncertainty in the predicted value due to noise on the target variables (expressed already in ML)

Uncertainty in the parameters $\mathbf{w}$ (consequence of Bayesian treatment)

Recap: Bayesian Predictive Distribution



- Important difference to previous example
  - Uncertainty may vary with test point x!

$$s(x)^2 = \beta^{-1} + \phi(x)^T \mathbf{S} \phi(x)$$

Image source: C.M. Bishop, 2006

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Loss Functions for Regression

- Given $p(y, \mathbf{x}, \mathbf{w}, \beta)$, how do we actually estimate a function value y_t for a new point $\mathbf{x}_t$?

- We need a loss function, just as in the classification case

$$
\begin{aligned}
L: \quad \mathbb{R} \times \mathbb{R} \quad &\rightarrow \quad \mathbb{R}^{+} \\
(t_n, y(\mathbf{x}_n)) \quad &\rightarrow \quad L(t_n, y(\mathbf{x}_n))
\end{aligned}
$$

- Optimal prediction: Minimize the expected loss

$$
\mathbb{E}[L] = \iint L(t, y(\mathbf{x})) p(\mathbf{x}, t) \,\mathrm{d}\mathbf{x} \,\mathrm{d}t
$$

Slide adapted from Stefan Roth

Loss Functions for Regression

$$\mathbb{E}[L] = \iint L(t, y(\mathbf{x}))p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

- Simplest case
  - Squared loss: $L(t, y(\mathbf{x})) = \{y(\mathbf{x}) - t\}^2$
  - Expected loss

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

$$\frac{\partial \mathbb{E}[L]}{\partial y(\mathbf{x})} = 2\int \{y(\mathbf{x}) - t\}\, p(\mathbf{x}, t)\mathrm{d}t \overset{!}{=} 0$$

$$\Leftrightarrow \int t p(\mathbf{x}, t)\mathrm{d}t = y(\mathbf{x}) \int p(\mathbf{x}, t)\mathrm{d}t$$

Slide adapted from Stefan Roth

Loss Functions for Regression

$$\int t p(\mathbf{x}, t)\mathrm{d}t \;=\; y(\mathbf{x}) \int p(\mathbf{x}, t)\mathrm{d}t$$

$$\Leftrightarrow\; y(\mathbf{x}) \;=\; \int t \frac{p(\mathbf{x}, t)}{p(\mathbf{x})}\mathrm{d}t = \int t p(t|\mathbf{x})\mathrm{d}t$$

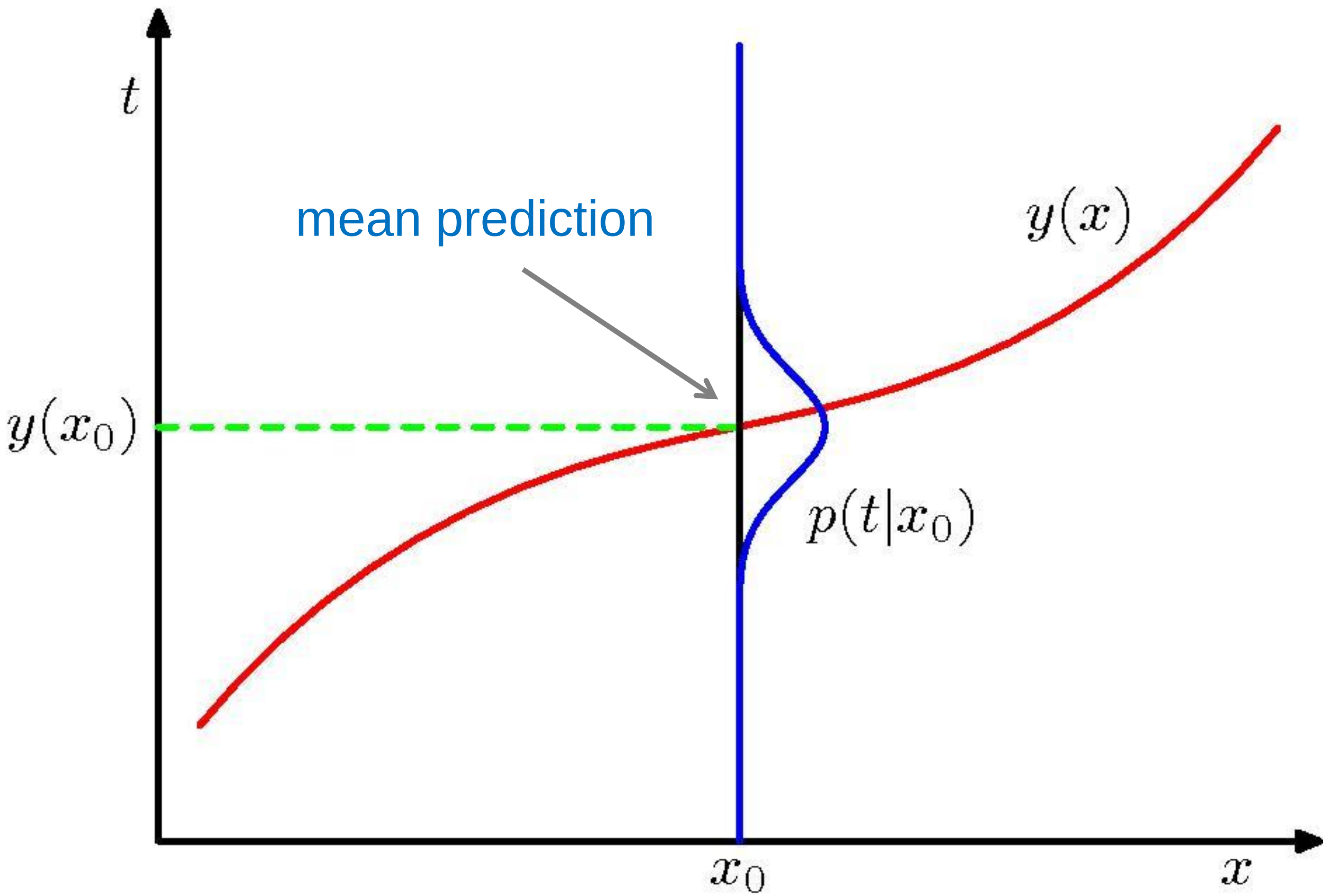
$$\Leftrightarrow\; y(\mathbf{x}) \;=\; \mathbb{E}[t|\mathbf{x}]$$

- Important result
  - Under Squared loss, the optimal regression function is the mean $\mathbb{E}\,[t|\mathbf{x}]$ of the posterior $p(t|\mathbf{x})$.
  - Also called mean prediction.
  - For our generalized linear regression function and square loss, we obtain as result

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

Slide adapted from Stefan Roth

Visualization of Mean Prediction



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Loss Functions for Regression

- Different derivation: Expand the square term as follows

$$
\begin{aligned}
\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] + \mathbb{E}[t|\mathbf{x}] - t\}^2 \\
&= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + \{\mathbb{E}[t|\mathbf{x}] - t\}^2 \\
&\quad + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\}
\end{aligned}
$$

- Substituting into the loss function
  - The cross-term vanishes, and we end up with

$$
\mathbb{E}[L] = \int \underbrace{\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2}\, p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int \underbrace{\mathrm{var}\left[t|\mathbf{x}\right]}\, p(\mathbf{x})\,\mathrm{d}\mathbf{x}
$$

Optimal least-squares predictor given by the conditional mean

Intrinsic variability of target data $\Rightarrow$ Irreducible minimum value of the loss function

Other Loss Functions

- The squared loss is not the only possible choice
  - Poor choice when conditional distribution $p(t|\mathbf{x})$ is multimodal.

- Simple generalization: Minkowski loss

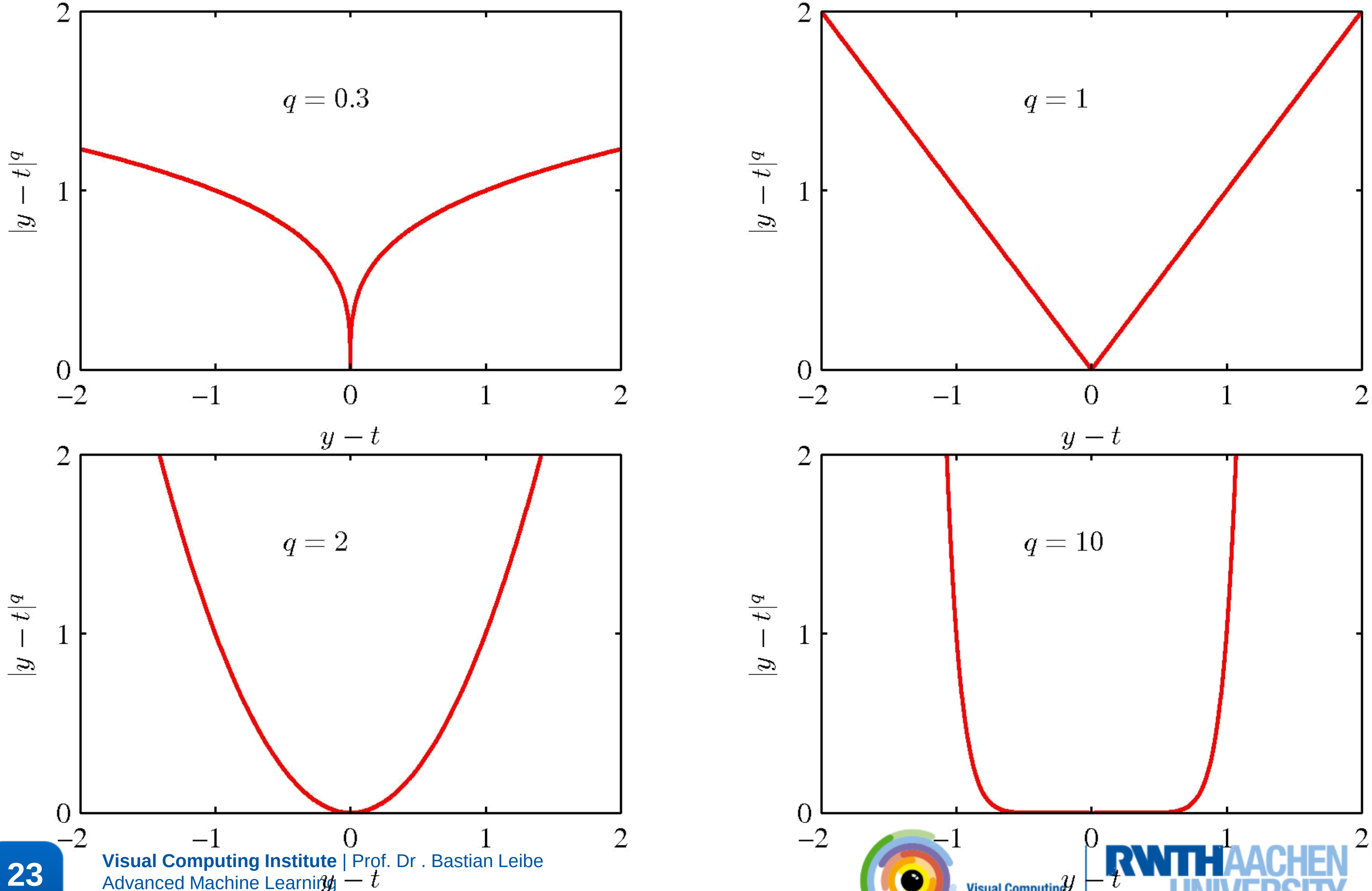
$$L(t, y(\mathbf{x})) = |y(\mathbf{x}) - t|^q$$

  - Expectation

$$\mathbb{E}[L_q] = \iint |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) \mathrm{d}\mathbf{x} \mathrm{d}t$$

- Minimum of $\mathbb{E}[L_q]$ is given by
  - Conditional mean for $q = 2$,
  - Conditional median for $q = 1$,
  - Conditional mode for $q = 0$.

Minkowski Loss Functions



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Linear Basis Function Models

- Generally, we consider models of the following form

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

  – where $\phi_j(\mathbf{x})$ are known as *basis functions*.
  – Typically, $\phi_0(\mathbf{x}) = 1$, so that w_0 acts as a bias.
  – In the simplest case, we use linear basis functions: $\phi_d(\mathbf{x}) = x_d$.

- *Let's take a look at some other possible basis functions...*

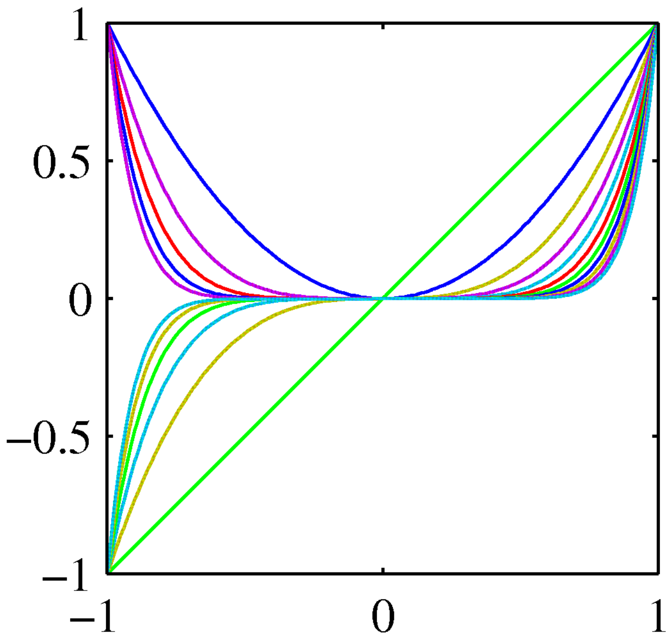
Slide adapted from C.M. Bishop, 2006

Linear Basis Function Models (2)

- Polynomial basis functions

$$\phi_j(x) = x^j.$$

- Properties
  - Global
    - $\Rightarrow$ A small change in x affects all basis functions.



Slide adapted from C.M. Bishop, 2006

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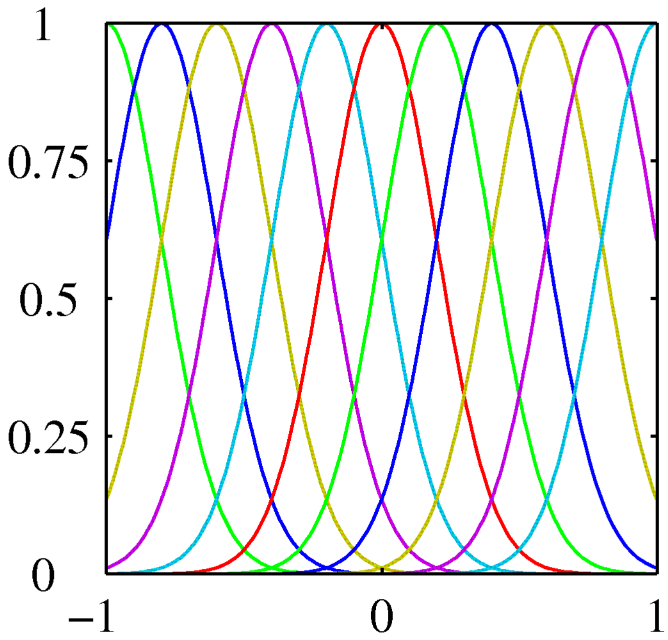
Linear Basis Function Models (3)

- Gaussian basis functions

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

- Properties
  - Local
    - $\Rightarrow$ A small change in x affects only nearby basis functions.
  - μ_j and s control location and scale (width).



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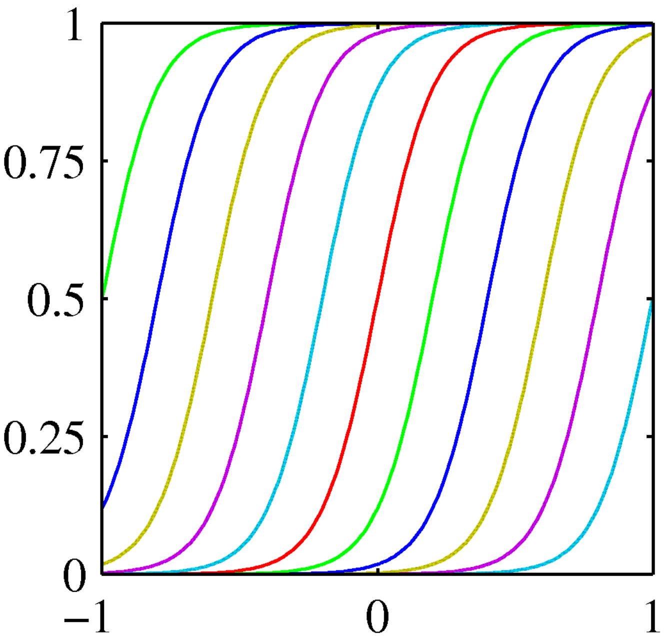
Linear Basis Function Models (4)

- Sigmoid basis functions

$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

  – where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$



- Properties
  – Local
  $\Rightarrow$ A small change in x affects only nearby basis functions.
  – μ_j and s control location and scale (slope).

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Multiple Outputs

- Multiple Output Formulation
  - So far only considered the case of a single target variable t.
  - We may wish to predict $K > 1$ target variables in a vector $\mathbf{t}$.
  - We can write this in matrix form

$$\mathbf{y}(\mathbf{x}, \mathbf{W}) = \mathbf{W}^T \phi(\mathbf{x})$$

  - where

$$\mathbf{y} = [y_1, \ldots, y_K]^T$$

$$\phi(\mathbf{x}) = [1, \phi_1(\mathbf{x}), \cdots, \phi_{M-1}(\mathbf{x}),]^T$$

$$\mathbf{W} = \begin{bmatrix} w_{0,1} & \cdots & w_{0,K} \\ \vdots & \ddots & \vdots \\ w_{M-1,1} & \cdots & w_{M-1,K} \end{bmatrix}^T$$

Multiple Outputs (2)

- Analogously to the single output case we have:

$$
\begin{aligned}
p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \beta) &= \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{W}, \mathbf{x}), \beta^{-1}\mathbf{I}) \\
&= \mathcal{N}(\mathbf{t}|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\mathbf{I}).
\end{aligned}
$$

- Given observed inputs, $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and targets, $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathbf{t}_N]^{\mathrm{T}}$, we obtain the log likelihood function

$$
\begin{aligned}
\ln p(\mathbf{T}|\mathbf{X}, \mathbf{W}, \beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\mathbf{I}) \\
&= \frac{NK}{2} \ln\left(\frac{\beta}{2\pi}\right) - \frac{\beta}{2} \sum_{n=1}^{N} \left\| \mathbf{t}_n - \mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) \right\|^2.
\end{aligned}
$$

Slide adapted from C.M. Bishop, 2006

Multiple Outputs (3)

- Maximizing with respect to $\mathbf{W}$, we obtain

$$\mathbf{W}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{T}.$$

- If we consider a single target variable, t_k, we see that

$$\mathbf{w}_k = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t}_k = \boldsymbol{\Phi}^{\dagger}\mathbf{t}_k$$

  – where $\mathbf{t}_k = [t_{1k}, \ldots, t_{Nk}]^{\mathrm{T}}$, which is identical with the single output case.

Slide adapted from C.M. Bishop, 2006

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Regularization Revisited

- Consider the error function

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization term

- With the sum-of-squares error function and a quadratic regularizer, we get

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

- which is minimized by

$$\mathbf{w} = \left(\lambda\mathbf{I} + \mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}.$$

λ is called the regularization coefficient.

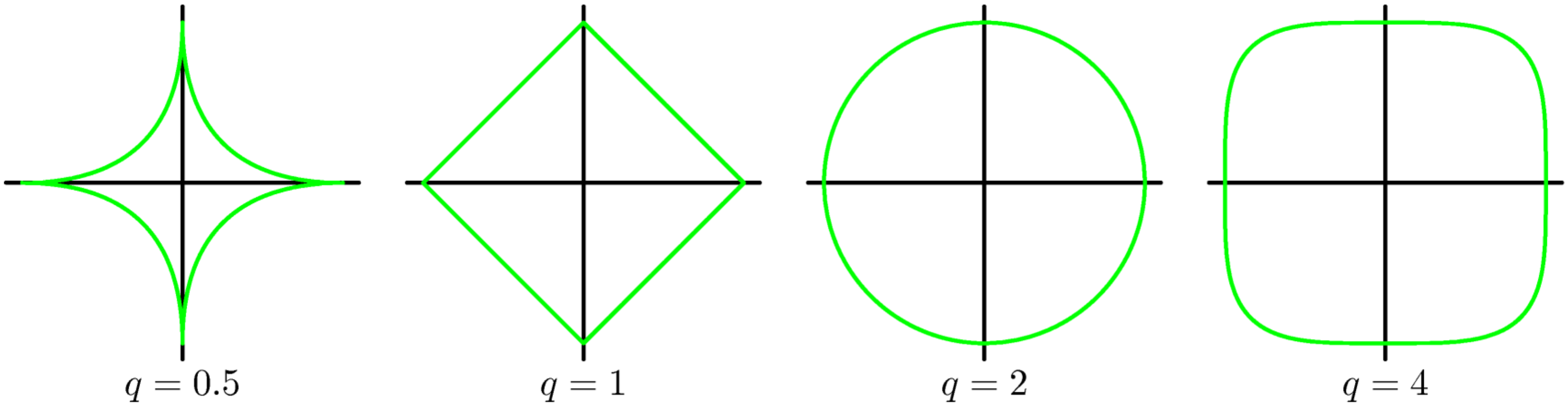
Slide adapted from C.M. Bishop, 2006

Regularized Least-Squares

- Let's look at more general regularizers

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

- "L_q norms"



"Lasso"

"Ridge Regression"

Slide adapted from C.M. Bishop, 2006

Image source: C.M. Bishop, 2006

Recall: Lagrange Multipliers

Regularized Least-Squares

- We want to minimize

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

- This is equivalent to minimizing

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

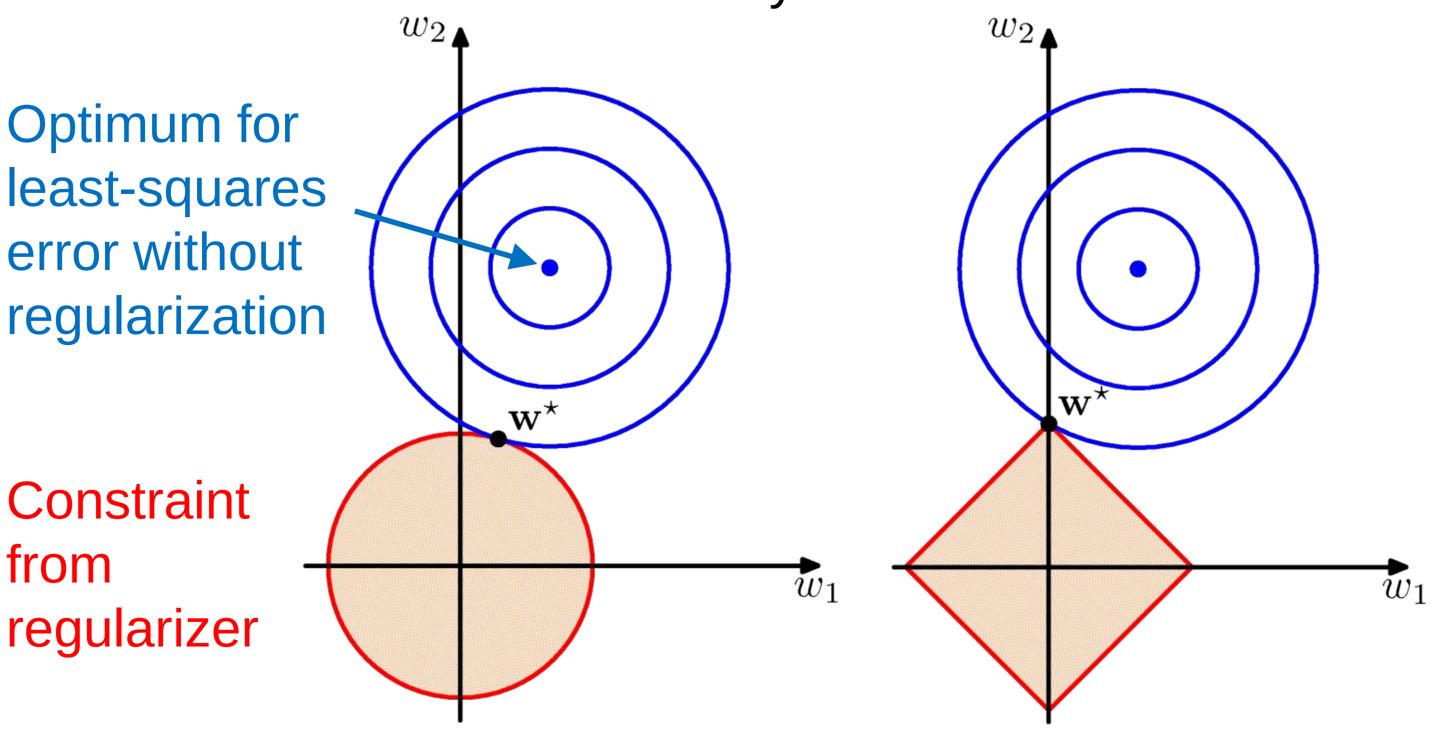
  – subject to the constraint

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

  – (for some suitably chosen η)

Regularized Least-Squares

- Effect: Sparsity for $q \leq 1$.
  - Minimization tends to set many coefficients to zero



  - *Why is this good?*
  - *Why don't we always do it, then? Any problems?*

Image source: C.M. Bishop, 2006

The Lasso

- Consider the following regressor

$$\mathbf{w}_{\text{Lasso}} = \arg\min_{\mathbf{w}} \; \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\}^2 + \lambda \sum_{j=1}^{M}|w_j|$$

  - This formulation is known as the Lasso.

- Properties
  - L_1 regularization $\Rightarrow$ The solution will be sparse (only few coefficients will be non-zero)
  - The L_1 penalty makes the problem non-linear.

  $\Rightarrow$ There is no closed-form solution.

  $\Rightarrow$ Need to solve a quadratic programming problem.
  - However, efficient algorithms are available with the same computational cost as for ridge regression.

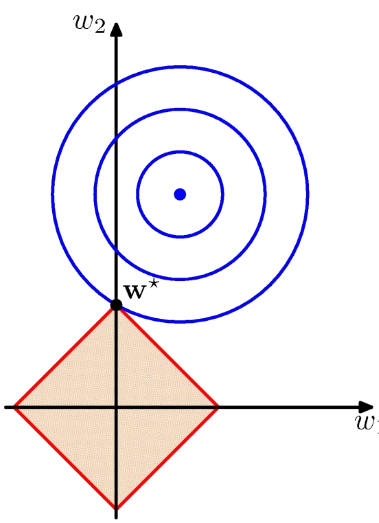


Image source: C.M. Bishop, 2006

Lasso as Bayes Estimation

- Interpretation as Bayes Estimation

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

  – We can think of $|w_j|^q$ as the log-prior density for w_j.

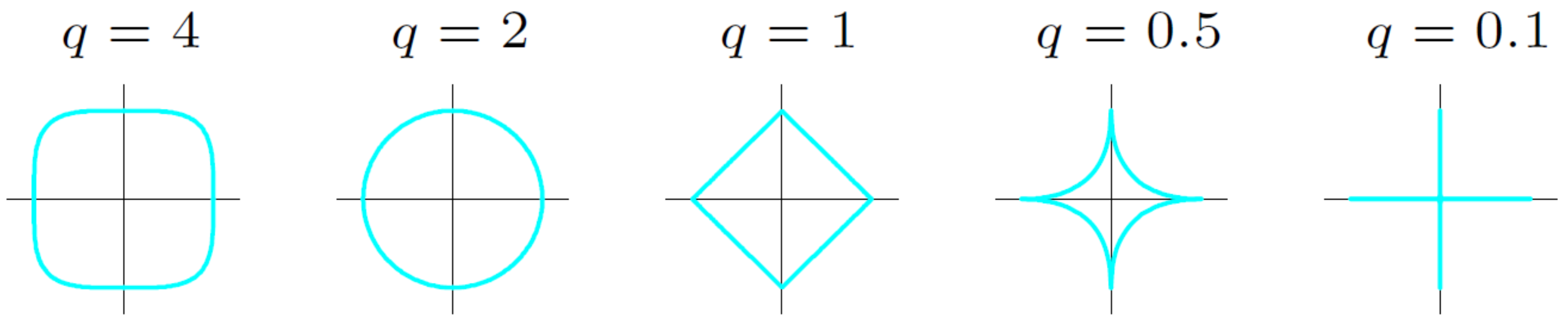
- Prior for Lasso ($q = 1$): Laplacian distribution

$$p(\mathbf{w}) = \frac{1}{2\tau}\exp\{-|\mathbf{w}|/\tau\} \qquad \text{with} \qquad \tau = \frac{1}{\lambda}$$

Image source: Friedman, Hastie, Tibshirani, 2009

Analysis

- Equicontours of the prior distribution



- Analysis
  - For $q \leq 1$, the prior is not uniform in direction, but concentrates more mass on the coordinate directions.
  - The case $q = 1$ (lasso) is the smallest q such that the constraint region is convex.

  $\Rightarrow$ Non-convexity makes the optimization problem more difficult.
  - Limit for $q = 0$: regularization term becomes $\sum_{j=1..M} 1 = M$.

  $\Rightarrow$ This is known as Best Subset Selection.

Image source: Friedman, Hastie, Tibshirani, 2009

Discussion

- Bayesian analysis
  - Lasso, Ridge regression and Best Subset Selection are Bayes estimates with different priors.
  - However, derived as maximizers of the posterior.
  - Should ideally use the posterior mean as the Bayes estimate!

  $\Rightarrow$ Ridge regression solution is also the posterior mean, but Lasso and Best Subset Selection are not.

- We might also try using other values of q besides $0,1,2\dots$
  - However, experience shows that this is not worth the effort.
  - Values of $q \in (1,2)$ are a compromise between lasso and ridge
  - However, $|w_j|^q$ with q > 1 is differentiable at 0.

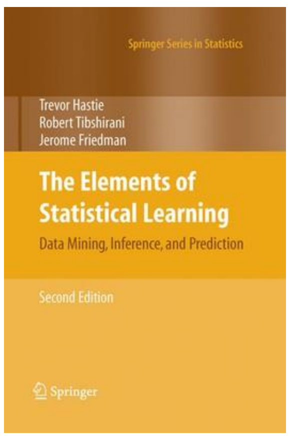
  $\Rightarrow$ Loses the ability of lasso for setting coefficients exactly to zero.

Topics of This Lecture

- Recap: Probabilistic View on Regression
- Properties of Linear Regression
  - Loss functions for regression
  - Basis functions
  - Multiple Outputs
- Regularization revisited
  - Regularized Least-squares
  - The Lasso
  - Discussion

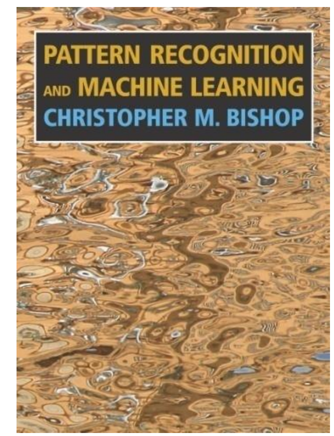
References and Further Reading

- More information on linear regression, including a discussion on regularization can be found in Chapters 1.5.5 and 3.1-3.2 of the Bishop book.



Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006

T. Hastie, R. Tibshirani, J. Friedman
Elements of Statistical Learning
2nd edition, Springer, 2009



- Additional information on the Lasso, including efficient algorithms to solve it, can be found in Chapter 3.4 of the Hastie book.