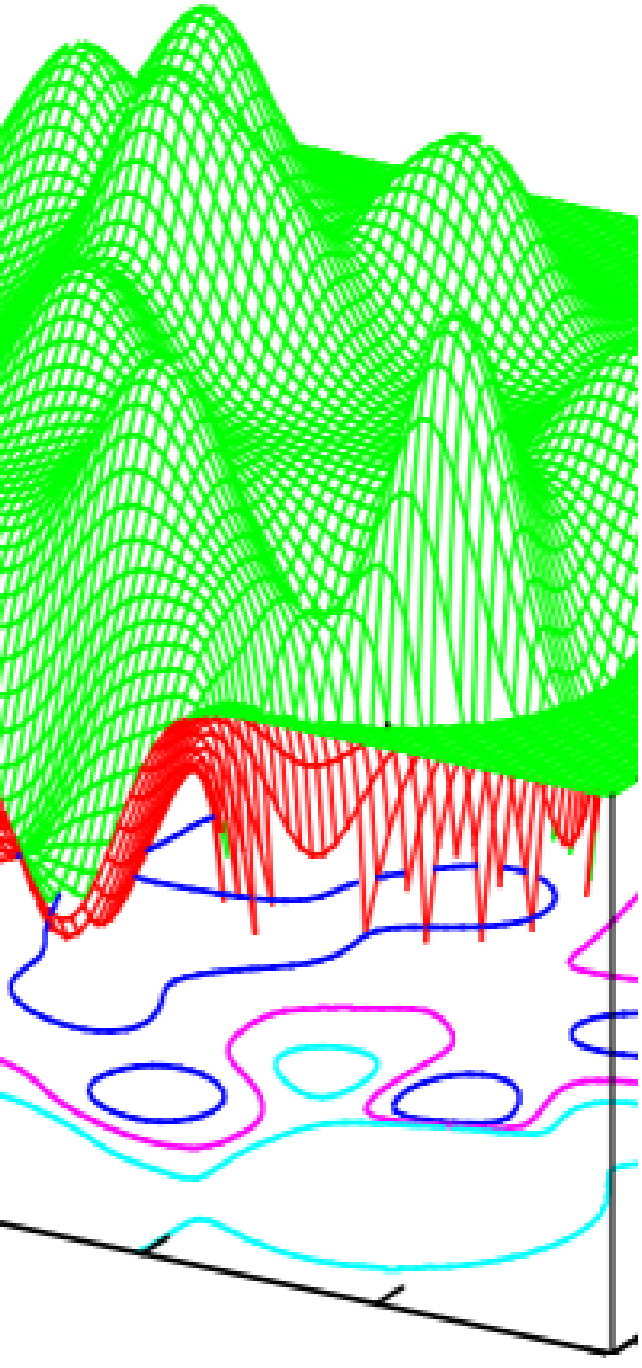

Machine Learning

Regression basics

Linear regression, non-linear features (polynomial, RBFs, piece-wise), regularization, cross validation, Ridge/Lasso, kernel trick

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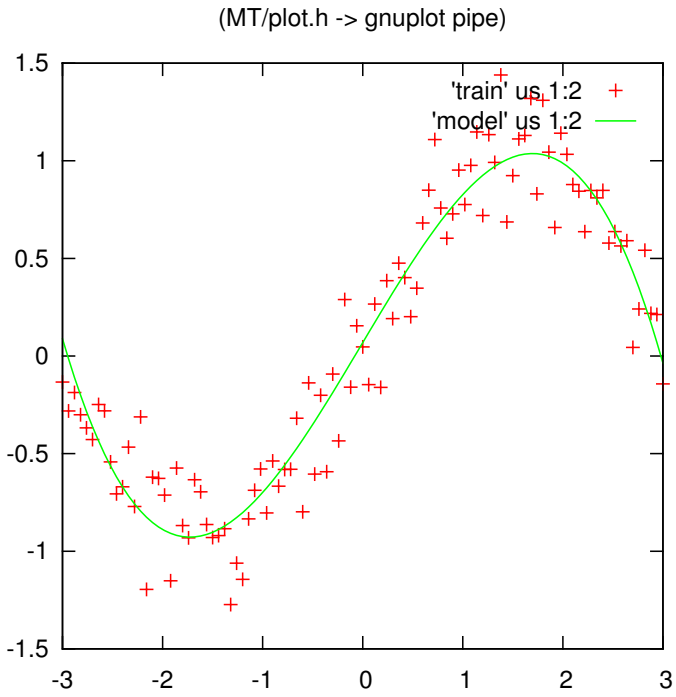
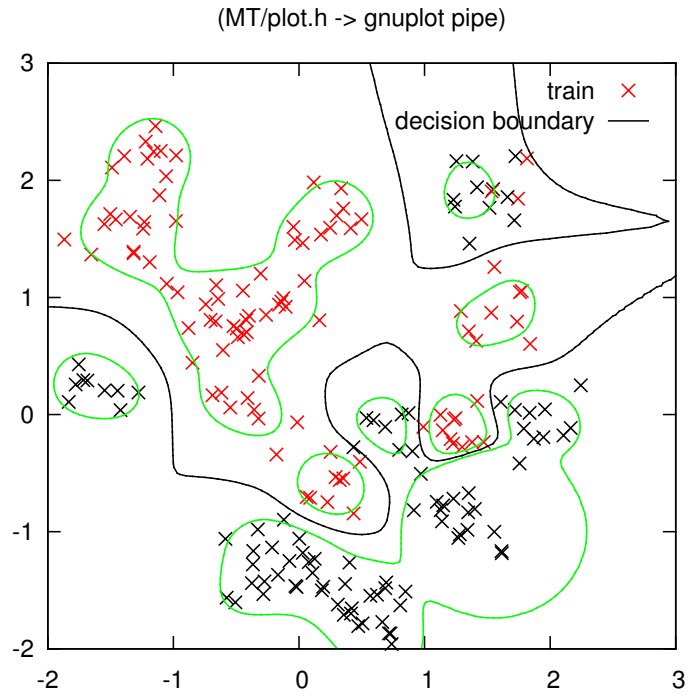
Summer 2014





- Are these linear models? Linear in *what*?
  - Input: No.
  - Parameters, features: Yes!

Linear Modelling is more powerful than it might seem at first!

Linear Modelling is more powerful than it might seem at first!

- Linear Regression on non-linear features $\rightarrow$ very powerful (polynomials, piece-wise, spline basis, kernels)
- Regularization (Ridge, Lasso) & cross-validation for proper generalization to test data
- Gaussian Processes and SVMs are closely related (linear in kernel features, but with different optimality criteria)
- Liquid/Echo State Machines, Extreme Learning, are examples of linear modelling on many (sort of random) non-linear features
- Basic insights in model complexity (effective degrees of freedom)
- Input relevance estimation (z-score) and feature selection (Lasso)
- Linear regression $\rightarrow$ linear classification (logistic regression: outputs are likelihood ratios)

$\Rightarrow$ Good foundation for learning about ML

(We roughly follow Hastie, Tibshirani, Friedman: *Elements of Statistical Learning*)

Linear Regression

- Notation:
  - input vector $x \in \mathbb{R}^d$
  - output value $y \in \mathbb{R}$
  - parameters $\beta = (\beta_0, \beta_1, .., \beta_d)^\top \in \mathbb{R}^{d+1}$
  - linear model

$$f(x) = \beta_0 + \sum_{j=1}^{d} \beta_j x_j$$

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$$f(x) = \beta_0 + \sum_{j=1}^{d} \beta_j x_j$$

- Given training data $D = \{(x_i, y_i)\}_{i=1}^n$ we define the *least squares* cost (or "loss")

$$L^{\text{ls}}(\beta) = \sum_{i=1}^{n} (y_i - f(x_i))^2$$

Optimal parameters β

- Augment input vector with a 1 in front:
  $\boldsymbol{x} = (1, x) = (1, x_1, .., x_d)^\top \in \mathbb{R}^{d+1}$
  $\beta = (\beta_0, \beta_1, .., \beta_d)^\top \in \mathbb{R}^{d+1}$

$$f(x) = \beta_0 + \sum_{j=1}^{n} \beta_j x_j = \boldsymbol{x}^\top \beta$$

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$$f(x) = \beta_0 + \sum_{j=1}^{n} \beta_j x_j = \boldsymbol{x}^\top \beta$$

- Rewrite sum of squares as:

$$L^{\mathsf{ls}}(\beta) = \sum_{i=1}^{n} (y_i - \boldsymbol{x}_i^\top \beta)^2 = \|y - \boldsymbol{X}\beta\|^2$$

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^\top \\ \vdots \\ \boldsymbol{x}_n^\top \end{pmatrix} = \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,d} \\ \vdots & & & & \vdots \\ 1 & x_{n,1} & x_{n,2} & \cdots & x_{n,d} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

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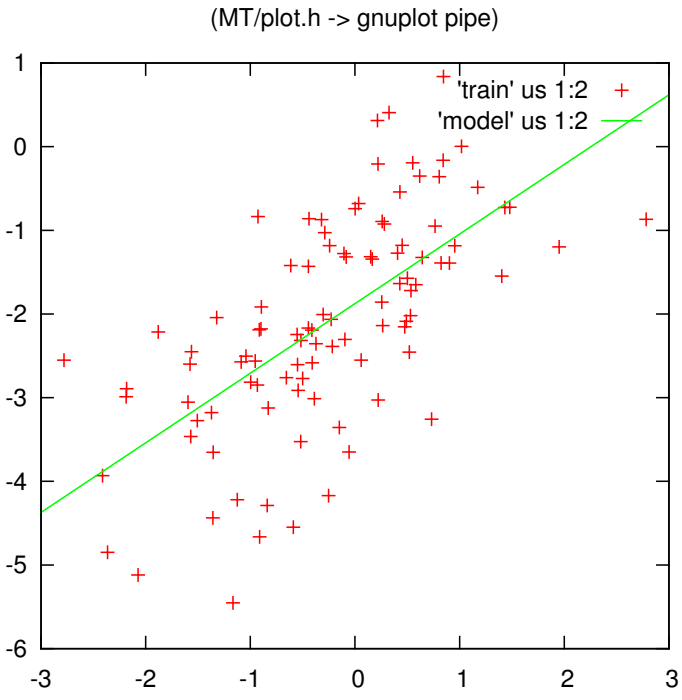
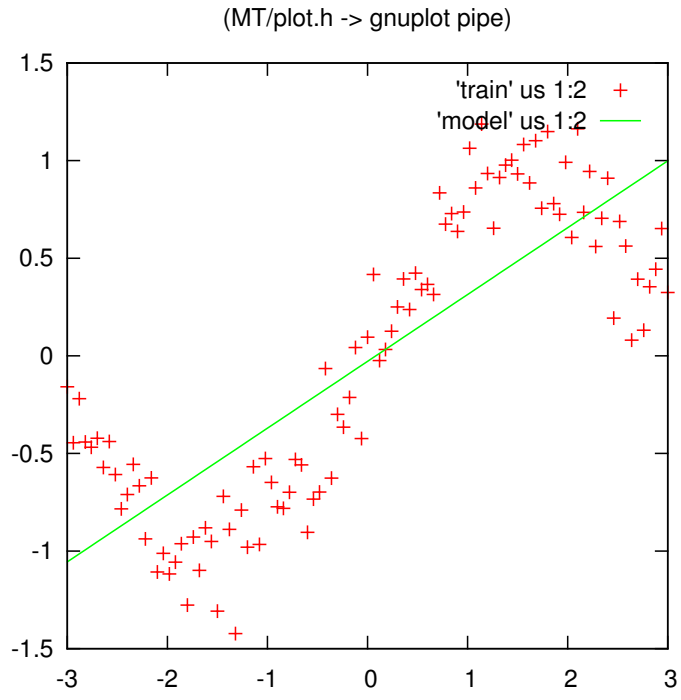
- Optimum:

$$\mathbf{0}_d^\top = \frac{\partial L^{\text{ls}}(\beta)}{\partial \beta} = -2(y - \boldsymbol{X}\beta)^\top \boldsymbol{X} \iff \mathbf{0}_d = \boldsymbol{X}^\top \boldsymbol{X}\beta - \boldsymbol{X}^\top y$$

$$\hat{\beta}^{\text{ls}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top y$$






```
./x.exe -mode 1 -dataFeatureType 1 -modelFeatureType 1
```

Non-linear features

- Replace the inputs $x_i \in \mathbb{R}^d$ by some non-linear features $\phi(x_i) \in \mathbb{R}^k$

$$f(x) = \sum_{j=1}^{k} \phi_j(x)\, \beta_j = \phi(x)^\top \beta$$

- The optimal β is the same

$$\hat{\beta}^{\text{ls}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y} \quad \text{but with} \quad \boldsymbol{X} = \begin{pmatrix} \phi(x_1)^\top \\ \vdots \\ \phi(x_n)^\top \end{pmatrix} \in \mathbb{R}^{n \times k}$$

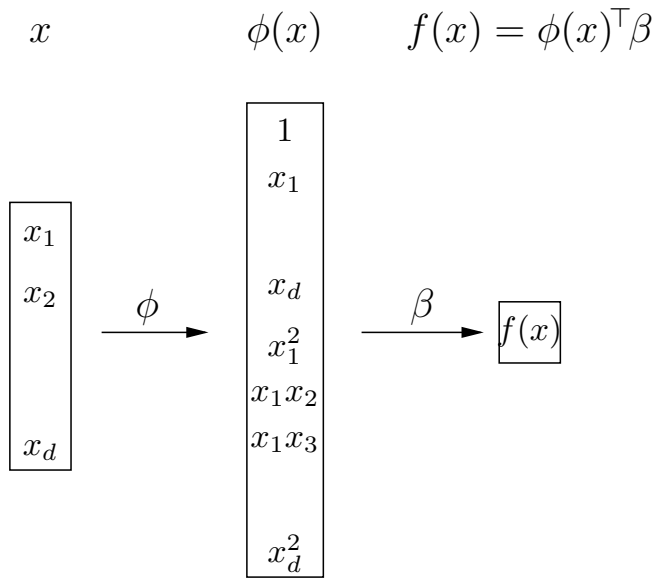
- What are "features"?

  a) Features are an arbitrary set of basis functions

  b) Any function *linear in* β can be written as $f(x) = \phi(x)^\top \beta$ for some ϕ—which we denote as "features"

Example: Polynomial features

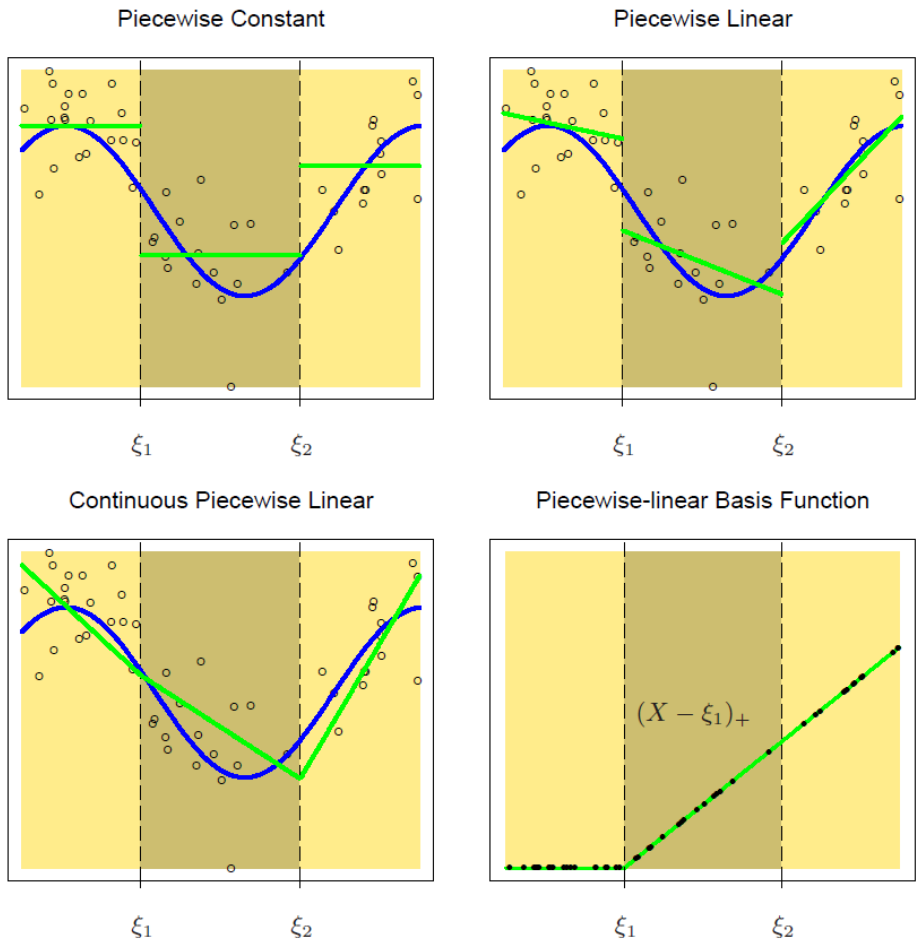
- Linear: $\phi(x) = (1, x_1, .., x_d) \in \mathbb{R}^{1+d}$
- Quadratic: $\phi(x) = (1, x_1, .., x_d, x_1^2, x_1x_2, x_1x_3, .., x_d^2) \in \mathbb{R}^{1+d+\frac{d(d+1)}{2}}$
- Cubic: $\phi(x) = (.., x_1^3, x_1^2x_2, x_1^2x_3, .., x_d^3) \in \mathbb{R}^{1+d+\frac{d(d+1)}{2}+\frac{d(d+1)(d+2)}{6}}$




```
./x.exe -mode 1 -dataFeatureType 1 -modelFeatureType 1
```

Example: Piece-wise features

- Piece-wise constant: $\phi_j(x) = I(\xi_1 < x < \xi_2)$
- Piece-wise linear: $\phi_j(x) = xI(\xi_1 < x < \xi_2)$
- Continuous piece-wise linear: $\phi_j(x) = (x - \xi_1)_+$



Example: Radial Basis Functions (RBF)

- Given a set of centers $\{c_j\}_{j=1}^k$, define

$$\phi_j(x) = b(x, c_j) = e^{-\frac{1}{2}\|x - c_j\|^2} \in [0, 1]$$

  Each $\phi_j(x)$ measures similarity with the center c_j

- Special case:

  use all training inputs $\{x_i\}_{i=1}^n$ as centers

$$\phi(x) = \begin{pmatrix} 1 \\ b(x, x_1) \\ \vdots \\ b(x, x_n) \end{pmatrix} \quad (n + 1 \text{ dim})$$

  This is related to "kernel methods" and GPs, but not quite the same—we'll discuss this later.

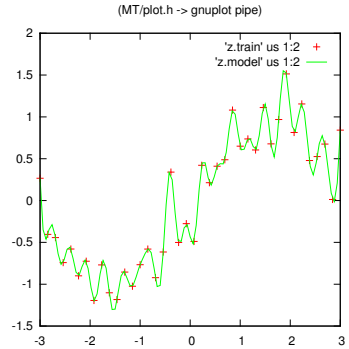
Features

- Polynomial
- Piece-wise
- Radial basis functions (RBF)
- Splines (see Hastie Ch. 5)

- Linear regression on top of rich features is extremely powerful!

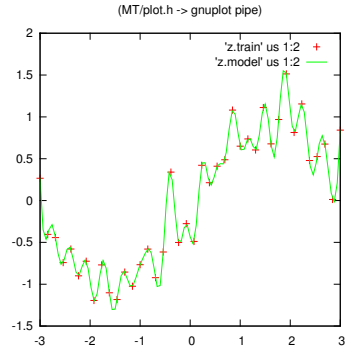
The need for regularization

Noisy $\sin$ data fitted with radial basis functions




```
./x.exe -mode 1 -n 40 -modelFeatureType 4 -dataType 2 -rbfWidth .1
-sigma .5 -lambda 1e-10
```

The need for regularization



Noisy $\sin$ data fitted with radial basis functions

```
./x.exe -mode 1 -n 40 -modelFeatureType 4 -dataType 2 -rbfWidth .1
-sigma .5 -lambda 1e-10
```

- **Overfitting & generalization:**
  The model overfits to the data—and generalizes badly

- **Estimator variance:**
  When you repeat the experiment (keeping the underlying function fixed), the regression always returns a different model estimate

Estimator variance

- Assumptions:
  – We computed parameters $\hat{\beta} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top y$
  – The data was noisy with variance $\text{Var}\{y\} = \sigma^2 \mathbf{I}_n$

  Then

  $$\text{Var}\{\hat{\beta}\} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \sigma^2$$

  – high data noise $\sigma \rightarrow$ high estimator variance
  – more data $\rightarrow$ less estimator variance: $\text{Var}\{\hat{\beta}\} \propto \frac{1}{n}$

- In practise we don't know σ, but we can estimate it based on the deviation from the learnt model:

$$\hat{\sigma}^2 = \frac{1}{n-d-1} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

Estimator variance

- "Overfitting"
  $\leftarrow$ picking one specific data set $y \sim \mathcal{N}(y_{\text{mean}}, \sigma^2 \mathbf{I}_n)$
  $\leftrightarrow$ picking one specific $\hat{b} \sim \mathcal{N}(\beta_{\text{mean}}, (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \sigma^2)$

- If we could reduce the variance of the estimator, we could reduce overfitting—and increase generalization.

Hastie's section on shrinkage methods is great! Describes several ideas on reducing estimator variance by reducing model complexity. We focus on regularization.

Ridge regression: L_2-regularization

- We add a *regularization* to the cost:

$$L^{\text{ridge}}(\beta) = \sum_{i=1}^{n} (y_i - \phi(x_i)^\top \beta)^2 + \lambda \sum_{j=1}^{k} \beta_j^2$$

NOTE: β_0 is usually *not* regularized!

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NOTE: β_0 is usually *not* regularized!

- Optimum:

$$\hat{\beta}^{\text{ridge}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda I)^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

(where $I = \mathbf{I}_k$, or with $I_{1,1} = 0$ if β_0 is not regularized)

- The objective is now composed of two “potentials”: The loss, which depends on the data and jumps around (introduces variance), and the regularization penalty (sitting steadily at zero). Both are “pulling” at the optimal $\beta \rightarrow$ the regularization reduces variance.

- The estimator variance becomes less: $\text{Var}\{\hat{\beta}\} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda I)^{-1} \sigma^2$

- The ridge effectively reduces the complexity of the model:

$$\text{df}(\lambda) = \sum_{j=1}^{d} \frac{d_j^2}{d_j^2 + \lambda}$$

where d_j^2 is the eigenvalue of $\boldsymbol{X}^\top \boldsymbol{X} = V D^2 V^\top$
(details: Hastie 3.4.1)

Choosing λ: generalization error & cross validation

- $\lambda = 0$ will always have a lower *training* data error
  We need to estimate the *generalization* error on test data

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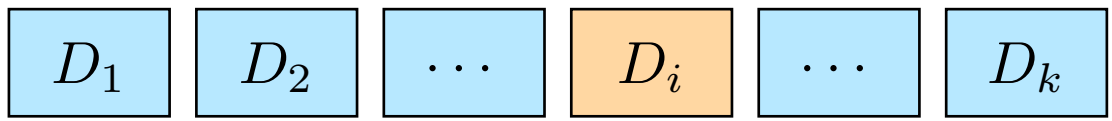
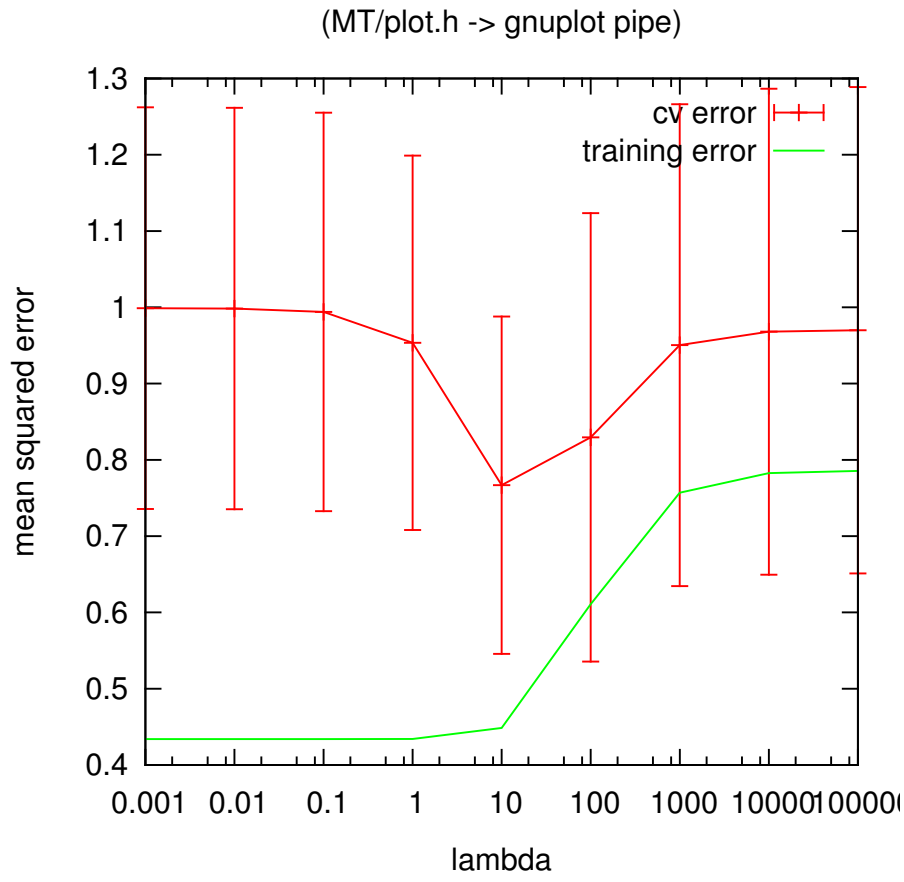
- *k-fold cross-validation:*



1: Partition data D in k equal sized subsets $D = \{D_1, .., D_k\}$
2: **for** $i = 1, .., k$ **do**
3: compute $\hat{\beta}_i$ on the training data $D \setminus D_i$ leaving out D_i
4: compute the error $\ell_i = L^{\text{ls}}(\hat{\beta}_i, D_i)$ on the validation data D_i
5: **end for**
6: report mean error $\hat{\ell} = 1/k \sum_i \ell_i$ and variance $(1/k \sum_i \ell_i^2) - \hat{\ell}^2$

- Choose λ for which $\hat{\ell}$ is smallest

quadratic features on sinus data:




```
./x.exe -mode 4 -n 10 -modelFeatureType 2 -dataType 2 -sigma .1
./x.exe -mode 1 -n 10 -modelFeatureType 2 -dataType 2 -sigma .1
```

Lasso: L_1-regularization

- We add a L_1 regularization to the cost:

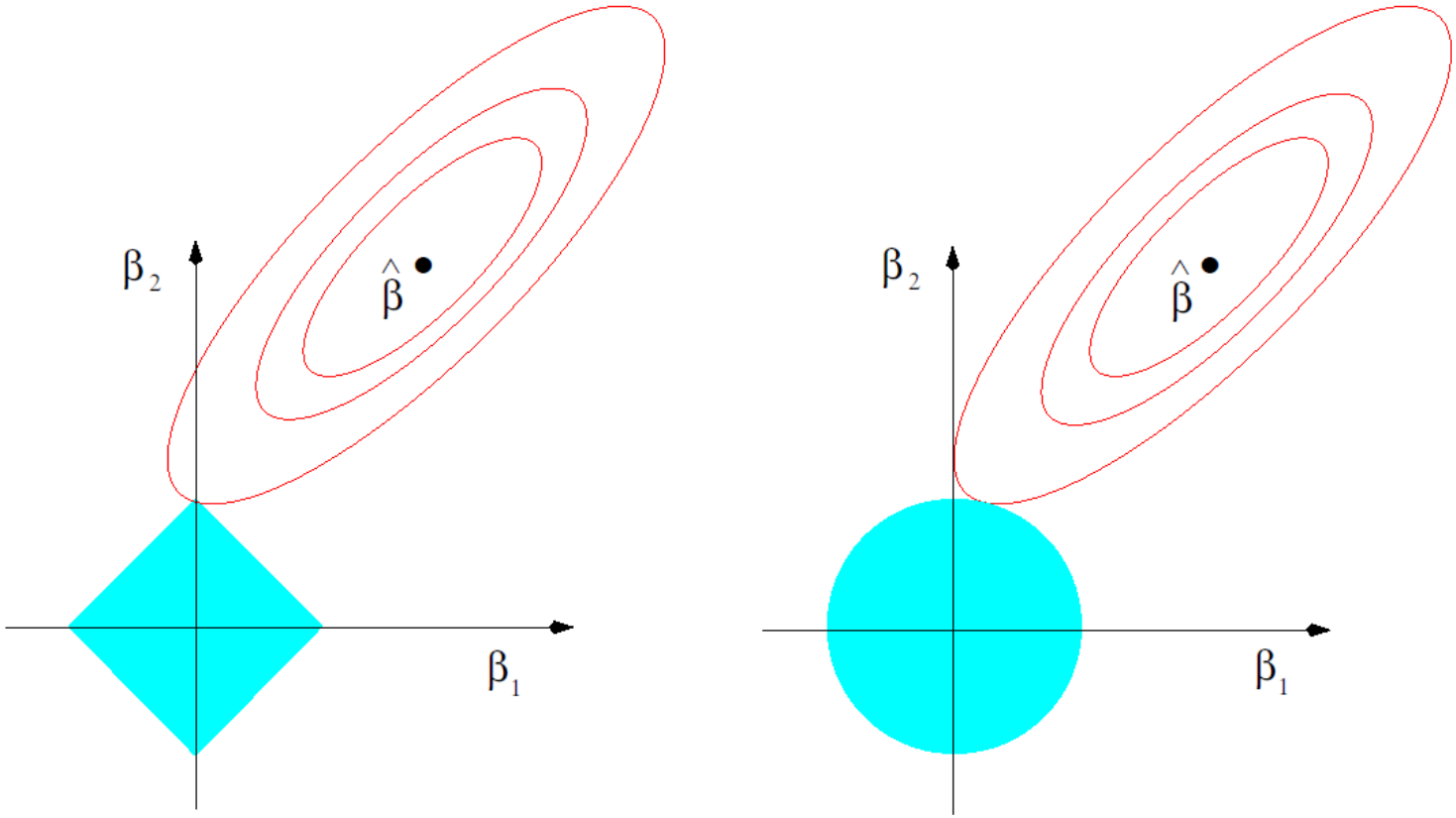
$$L^{\text{lasso}}(\beta) = \sum_{i=1}^{n} (y_i - \phi(x_i)^\top \beta)^2 + \lambda \sum_{j=1}^{k} |\beta_j|$$

  NOTE: β_0 is usually not regularized!

- Has no closed form expression for optimum

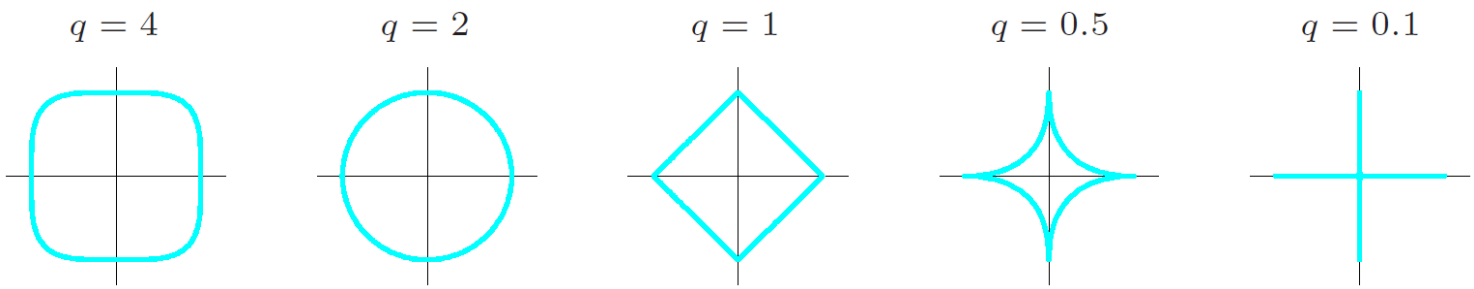
  (Optimum can be found by solving a quadratic program; see appendix.)

Lasso vs. Ridge:



- Lasso $\rightarrow$ sparsity! feature selection!

$$L^q(\beta) = \sum_{i=1}^{n} (y_i - \phi(x_i)^\top \beta)^2 + \lambda \sum_{j=1}^{k} |\beta_j|^q$$



- *Subset selection:* $q = 0$ (counting the number of $\beta_j \neq 0$)

Summary

- **Linear models** on non-linear features—extremely powerful

linear polynomial RBF kernel	Ridge Lasso	regression classification

- Generalization $\leftrightarrow$ **Regularization** $\leftrightarrow$ complexity/DoF penalty

- **Cross validation** to estimate generalization empirically $\rightarrow$ use to choose regularization parameters

Kernel Ridge Regression—the "Kernel Trick"

- Reconsider solution of Ridge regression:

$$\hat{\beta}^{\text{ridge}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \mathbf{I}_k)^{-1} \boldsymbol{X}^\top \boldsymbol{y} = \boldsymbol{X}^\top (\boldsymbol{X}\boldsymbol{X}^\top + \lambda \mathbf{I}_n)^{-1} \boldsymbol{y}$$

Kernel Ridge Regression—the "Kernel Trick"

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$$\hat{\beta}^{\text{ridge}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \mathbf{I}_k)^{-1} \boldsymbol{X}^\top \boldsymbol{y} = \boldsymbol{X}^\top (\boldsymbol{X}\boldsymbol{X}^\top + \lambda \mathbf{I}_n)^{-1} \boldsymbol{y}$$

- Recall $\boldsymbol{X}^\top = (\phi(x_1), .., \phi(x_n)) \in \mathbb{R}^{k \times n}$, then:

$$f^{\text{ridge}}(x) = \phi(x)^\top \beta^{\text{ridge}} = \underbrace{\phi(x)^\top \boldsymbol{X}^\top}_{\boldsymbol{\kappa}(x)} (\underbrace{\boldsymbol{X}\boldsymbol{X}^\top}_{\boldsymbol{K}} + \lambda I)^{-1} \boldsymbol{y}$$

$\boldsymbol{K}$ is called *kernel matrix* and has elements

$$\boldsymbol{K}_{ij} = k(x_i, x_j) := \phi(x_i)^\top \phi(x_j)$$

$\boldsymbol{\kappa}$ is the row vector: $\boldsymbol{\kappa}(x) = k(x, x_{1:n}) = \phi(x)^\top \boldsymbol{X}^\top$.

The kernel function $k(x, x')$ calculates the scalar product in feature space.

The Kernel Trick

- We can rewrite kernel ridge regression as:

$$f^{\text{rigde}}(x) = \boldsymbol{\kappa}(x)(\boldsymbol{K} + \lambda I)^{-1}\boldsymbol{y}$$
$$\text{with } \boldsymbol{K}_{ij} = k(x_i, x_j)$$
$$\boldsymbol{\kappa}_i(x) = k(x, x_i) \quad \text{(a row vector)}$$

  $\rightarrow$ at no place we actually need to compute the parameters $\hat{\beta}$
  $\rightarrow$ at no place we actually need to compute the features $\phi(x_i)$
  – we only need to be able to compute $k(x, x')$ for any x, x'

- This rewriting is called *kernel trick.*
- It has great implications:
  – Instead of inventing funny non-linear features, we may directly invent funny kernels
  – Inventing a kernel is intuitive: $k(x, x')$ expresses how correlated y and y' should be: it is a meassure of similarity, it compares x and x'. Specifying how 'comparable' x and x' are is often more intuitive than defining "features that might work".

- Every choice of features implies a kernel. But,

Does every choice of kernel correspond to specific choice of feature?

Reproducing Kernel Hilbert Space

- Let's define a vector space $\mathcal{H}_k$, spanned by infinitely many basis elements

$$\{h_x = k(\cdot, x) \ : \ x \in \mathbb{R}^d\}$$

  Vectors in this space are linear combinations of such basis elements, e.g.,

$$f = \sum_i \alpha_i h_{x_i} \ , \quad f(x) = \sum_i \alpha_i k(x, x_i)$$

- Let's define a scalar product in this space, by first defining the scalar product for every basis element,

$$\langle h_x, h_y \rangle := k(x, y)$$

  This is positive definite. Note, it follows

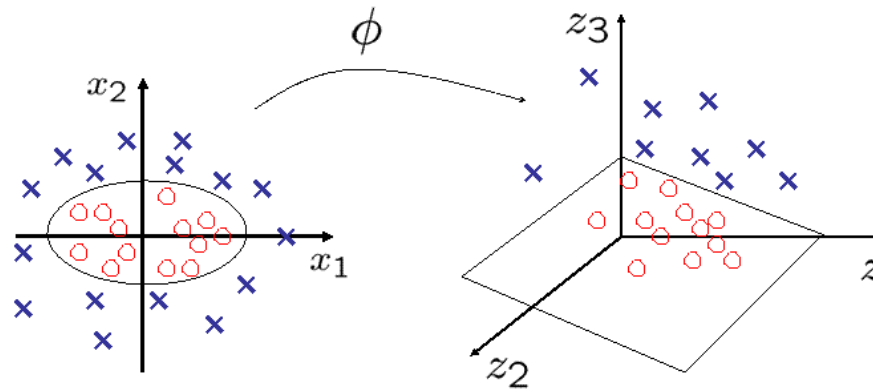
$$\langle h_x, f \rangle = \sum_i \alpha_i \langle h_x, h_{x_i} \rangle = \sum_i \alpha_i k(x, x_i) = f(x)$$

- The $\phi(x) = h_x = k(\cdot, x)$ is the 'feature' we associate with x. Note that this is a function and infinite dimensional.
  Choosing $\boldsymbol{\alpha} = (\boldsymbol{K} + \lambda I)^{-1}\boldsymbol{y}$ represents $f^{\text{ridge}}(x) = \sum_{i=1}^n \alpha_i k(x, x_i)$, and shows that ridge regression has a finite-dimensional solution in the basis elements $\{h_{x_i}\}$. A more general version of this insight is called **representer theorem**.

Example Kernels

- Kernel functions need to be positive definite: $\forall_{z:|z|>0} : k(z, z') > 0$
  $\rightarrow \boldsymbol{K}$ is a positive definite matrix
- Examples:
  - Polynomial: $k(x, x') = (x^\top x')^d$
    $d = 2, x \in \mathbb{R}^2$, $\phi(x) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)^\top$

$$k(x, x') = ((x_1, x_2)\begin{pmatrix} x_1' \\ x_2' \end{pmatrix})^2$$
$$= (x_1x_1' + x_2x_2')^2$$
$$= x_1^2{x_1'}^2 + 2x_1x_2x_1'x_2' + x_2^2{x_2'}^2$$
$$= (x_1^2, \sqrt{2}x_1x_2, x_2^2)({x_1'}^2, \sqrt{2}x_1'x_2', {x_2'}^2)^\top$$
$$= \phi(x)^\top\phi(x')$$



  - Gaussian (radial basis function): $k(x, x') = \exp(-\gamma \,|\, x - x' \,|\, ^2)$

Appendix: Alternative formulation of Ridge

- The standard way to write the Ridge regularization:

$$L^{\text{ridge}}(\beta) = \sum_{i=1}^{n}(y_i - \phi(x_i)^\top\beta)^2 + \lambda\sum_{j=1}^{k}\beta_j^2$$

- Finding $\hat{\beta}^{\text{ridge}} = \text{argmin}_\beta\, L^{\text{ridge}}(\beta)$ is equivalent to solving

$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\text{argmin}} \sum_{i=1}^{n}(y_i - \phi(x_i)^\top\beta)^2$$

$$\text{subject to } \sum_{j=1}^{k}\beta_j^2 \leq t$$

λ is the Lagrange multiplier for the inequality constraint

Appendix: Alternative formulation of Lasso

- The standard way to write the Lasso regularization:

$$L^{\text{lasso}}(\beta) = \sum_{i=1}^{n}(y_i - \phi(x_i)^\top\beta)^2 + \lambda\sum_{j=1}^{k}|\beta_j|$$

- Equivalent formulation (via KKT):

$$\hat{\beta}^{\text{lasso}} = \operatorname*{argmin}_{\beta} \sum_{i=1}^{n}(y_i - \phi(x_i)^\top\beta)^2$$

$$\text{subject to } \sum_{j=1}^{k}|\beta_j| \leq t$$

- Decreasing t is called "shrinkage": The space of allowed β shrinks. Some β will become zero $\rightarrow$ feature selection