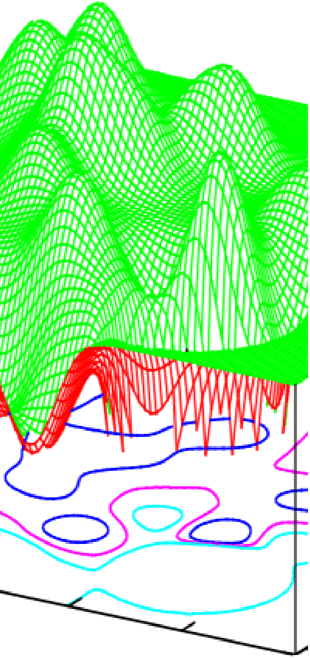

Machine Learning

Regression basics

Marc Toussaint
University of Stuttgart
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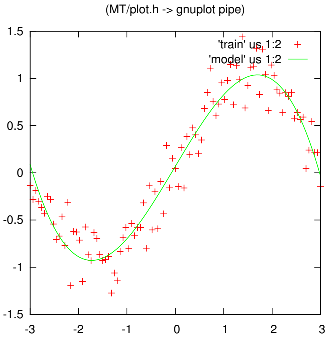

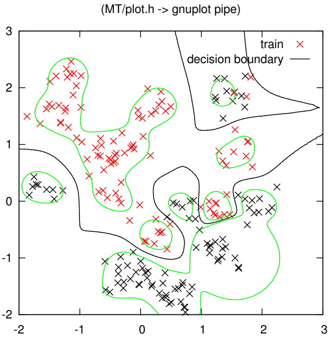

- Are these linear models? Linear in *what*?
  - – Input: No.
  - – Parameters, features: Yes!

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 → 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 → linear classification (logistic regression: outputs are likelihood ratios)

$\Rightarrow$ Linear modelling is a core of 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:
  $\bar{x} = (1, x) = (1, x_1, .., x_d)^\top \in \mathbb{R}^{d+1}$
  $\beta = (\beta_0, \beta_1, .., \beta_d)^\top \in \mathbb{R}^{d+1}$

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

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

- Rewrite sum of squares as:
  $$L^{\text{ls}}(\beta) = \textstyle\sum_{i=1}^n (y_i - \bar{x}_i^\top \beta)^2 = \|y - X\beta\|^2$$

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

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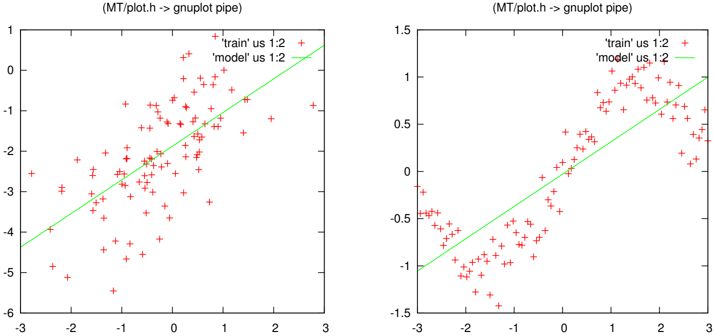
- Optimum:
  $\mathbf{0}_d^\top = \frac{\partial L^{\text{ls}}(\beta)}{\partial \beta} = -2(y - X\beta)^\top X \iff \mathbf{0}_d = X^\top X \beta - X^\top y$
  $$\boxed{\hat{\beta}^{\text{ls}} = (X^\top X)^{\text{-}1} X^\top y}$$



```
./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

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

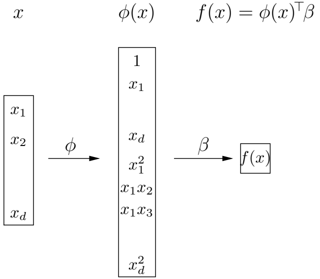
- What are "features"?

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



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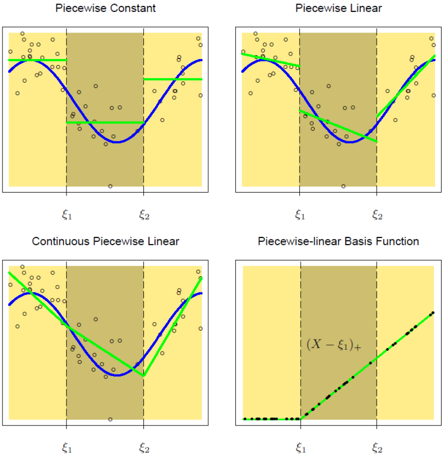
./x.exe -mode 1 -dataFeatureType 1 -modelFeatureType 1
```

Example: Piece-wise features

- Piece-wise constant: $\phi_j(x) = [\xi_1 < x < \xi_2]$
- Piece-wise linear: $\phi_j(x) = x\,[\xi_1 < x < \xi_2]$
- 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

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

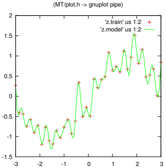
  This is related to "kernel methods" and GPs, but not quite the same—we'll discuss this later.

Features

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

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

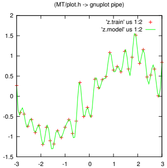
The need for regularization



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

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

  Then

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

  – high data noise σ → high estimator variance
  – more data → 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 $\hat{b} \sim \mathcal{N}(\beta_{\text{mean}}, (X^\top X)^{\text{-1}} \sigma^2)$

- 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:

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

NOTE: β_1 is usually *not* regularized!

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NOTE: β_1 is usually *not* regularized!

- Optimum:

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

(where $I = \mathbf{I}_k$, or with $I_{1,1} = 0$ if β_1 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: Var$\{\hat{\beta}\} = (X^\top X + \lambda I)^{\text{-1}} \sigma^2$

- The ridge effectively reduces the complexity of the model:

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

  where d_j^2 is the eigenvalue of $X^\top X = V D^2 V^\top$
  (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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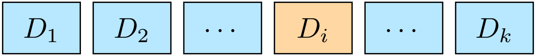
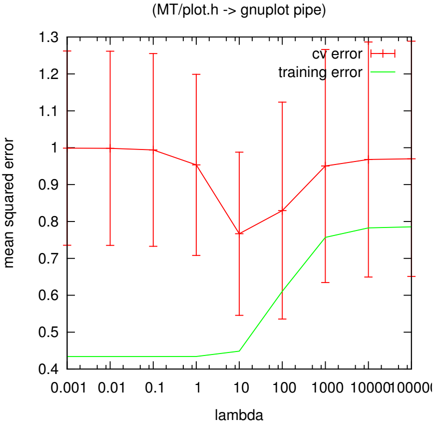
- k*-fold cross-validation:*



D_1 D_2 $\cdots$ D_i $\cdots$ D_k

```
Partition data $D$ in $k$ equal sized subsets $D = \{D_1, .., D_k\}$
for $i = 1, .., k$ do
    compute $\hat\beta_i$ on the training data $D \setminus D_i$ leaving out $D_i$
    compute the error $\ell_i = L^{\text{ls}}(\hat\beta_i, D_i)$ on the validation data $D_i$
end for
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:

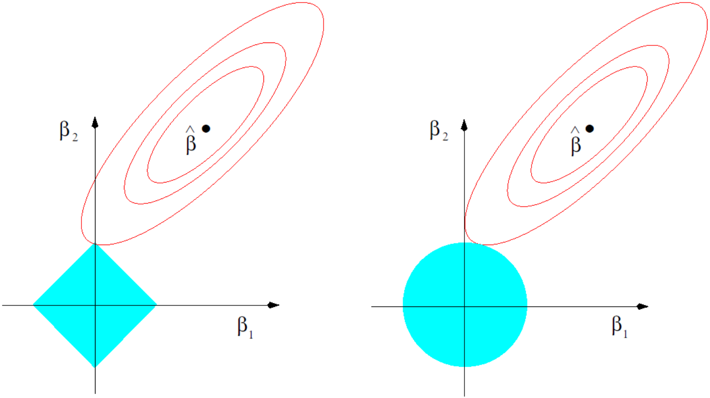
$$L^{\text{lasso}}(\beta) = \sum_{i=1}^n (y_i - \phi(x_i)^\top \beta)^2 + \lambda \sum_{j=1}^k |\beta_j|$$

NOTE: β_1 is usually not regularized!

- Has no closed form expression for optimum

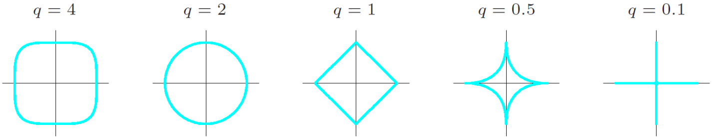
(Optimum can be found by solving a quadratic program; see appendix.)

Lasso vs. Ridge:



- Lasso → 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

- **Representation:** choice of features

$$f(x) = \phi(x)^\top \beta$$

- **Objective:** squared error + Ridge/Lasso regularization

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

- **Solver:** analytical (or quadratic program for Lasso)

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

Summary

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

linear polynomial RBF kernel	Ridge Lasso	regression classification*

*logistic regression

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

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

Appendix: Dual 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 $\hat{\beta}^{\text{ridge}} = \operatorname{argmin}_\beta L^{\text{ridge}}(\beta)$ is equivalent to solving

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

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

λ is the Lagrange multiplier for the inequality constraint

Appendix: Dual formulation of Lasso

- The standard way to write the Lasso regularization:
$$L^{\text{lasso}}(\beta) = \textstyle\sum_{i=1}^n (y_i - \phi(x_i)^\top \beta)^2 + \lambda \sum_{j=1}^k |\beta_j|$$

- Equivalent formulation (via KKT):
$$\hat\beta^{\text{lasso}} = \operatorname*{argmin}_\beta \sum_{i=1}^n (y_i - \phi(x_i)^\top \beta)^2$$
$$\text{subject to } \sum_{j=1}^k |\beta_j| \le t$$

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