Intro to Regression

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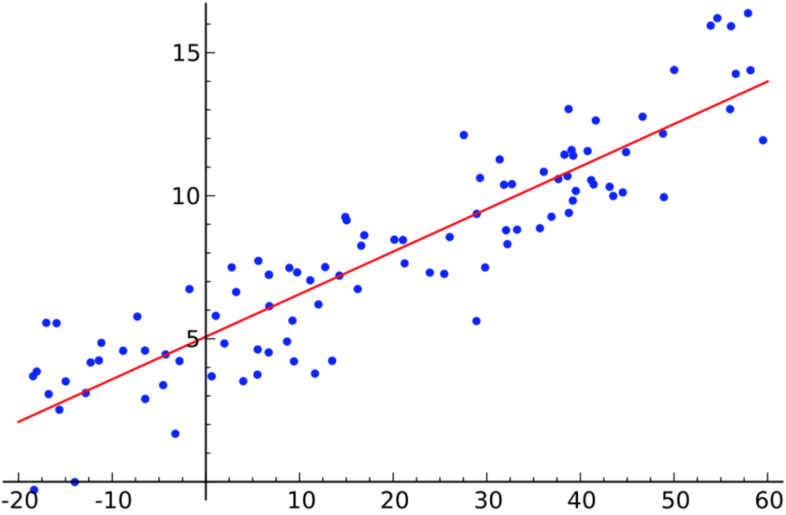
Outline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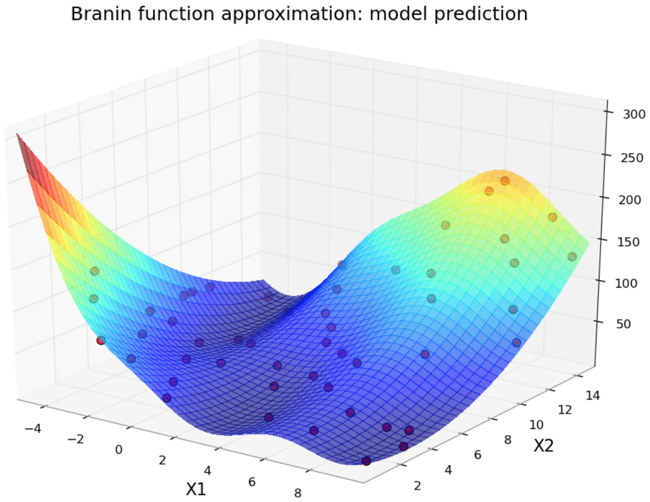
Branin function approximation: model prediction
300
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6
8
X1
2
4
6
8
10
12
14
X2

- **Training data**: sample drawn i.i.d. from set X according to some distribution D

$$S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\} \in X \times Y,$$

with $Y \subseteq \mathbb{R}$ is a measurable set, $X \subseteq \mathbb{R}^d$, $\mathbf{x}_i \in \mathbb{R}^{1 \times d}$

- **Loss function**: $L : Y \times Y \to \mathbb{R}_+$ a measure of closeness, e.g. $L(y, y') = (y - y')^2$ or $L(y, y') = |y - y'|^p$ for some $p \geq 1$

- **Problem**: find hypothesis $\widehat{f} : X \to \mathbb{R}$ in $\mathbb{H}$ with small generalization error w.r.t. target f

$$R_D(\widehat{f}) = \mathbb{E}_{\mathbf{x} \sim D}[L(\widehat{f}(\mathbf{x}), f(\mathbf{x}))]$$

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- Empirical error:

$$\widehat{R}_D(h) = \frac{1}{m}\sum_{i=1}^{m} L(\widehat{f}(\mathbf{x}_i), y_i)$$

- In much of what follows:
  - $Y = \mathbb{R}$ or $Y = [-M, M]$ for some $M > 0$
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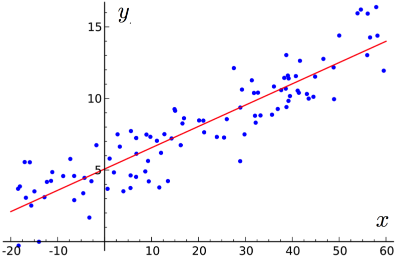
- **Object** $\mathbf{x}$: place to open a new restaurant
- **Label** y: revenue after one year of operation
- **Features**: demographic properties of a considered city district, prices for real estate in a local neighborhood, availability of offices nearby, etc.
- **Challenges**:
  - small sample size
  - a lot of features ($d \gg 1$)
  - outliers/incorrect measurements
  - non-homogeneous data (big cities vs. local towns)

- Hypothesis set: linear functions

$$\mathbb{H} = \{\mathbf{x} \to \mathbf{w} \cdot \mathbf{x}^{\mathrm{T}} + b : \mathbf{w} \in \mathbb{R}^{1 \times d}, b \in \mathbb{R}\}$$

- **Optimization problem**: empirical risk minimization

$$F(\mathbf{w}, b) = \frac{1}{m} \sum_{i=1}^{m} \left(\mathbf{w} \cdot \mathbf{x}_i^{\top} + b - y_i\right)^2 \to \min_{\mathbf{w}, b}$$



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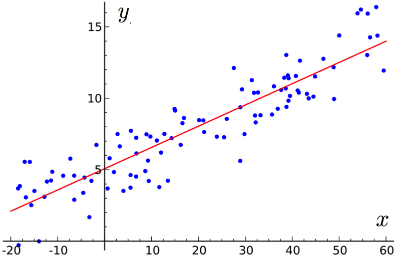

- Rewrite objective function as $F(\mathbf{W}) = \frac{1}{m}\|\mathbf{X}\mathbf{W} - \mathbf{Y}\|^2$, where

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & 1 \\ \vdots & \vdots \\ \mathbf{x}_m & 1 \end{bmatrix} \in \mathbb{R}^{m\times(d+1)},\ \mathbf{W} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \\ b \end{bmatrix},\ \mathbf{Y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

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- **Solution**:

$$\mathbf{W} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \text{ if } \mathbf{X}^\top \mathbf{X} \text{ invertible}$$

- Computational complexity: $O(md + d^3)$ if matrix inversion is in $O(d^3)$
- Poor guarantees in general, no regularization
- For output labels in $\mathbb{R}^{d_y}$, $d_y > 1$, solve d_y distinct linear regression problems

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- **Optimization problem**:

$$F(\mathbf{w}, b) = \sum_{i=1}^{m} (\mathbf{w} \cdot \mathbf{x}_i^\top + b - y_i)^2 + \lambda \|\mathbf{w}\|^2 \to \min_{\mathbf{w}, b},$$

where $\lambda \geq 0$ is a regularization parameter

- **Benefits**:
  - directly based on generalization bound (strict result!)
  - generalization of linear regression
  - closed-form solution
  - can be used with kernels (next slides!)

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- Rewrite objective function as

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Ridge Regression: Solution

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$$\nabla F(\mathbf{W}) = 2\lambda\mathbf{W} + 2\mathbf{X}^\top(\mathbf{X}\mathbf{W} - \mathbf{Y})$$

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Type	Solution	Prediction
Primal	$O(md^2 + d^3)$	$O(d)$
Dual	$O(\varkappa m^2 + m^3)$	$O(\varkappa m)$

Here $\varkappa$ denotes the time complexity of computing a dot product; Euclidian dot product $\varkappa = O(d)$

- **Optimization problem**: "Least Absolute Shrinkage and Selection Operator"

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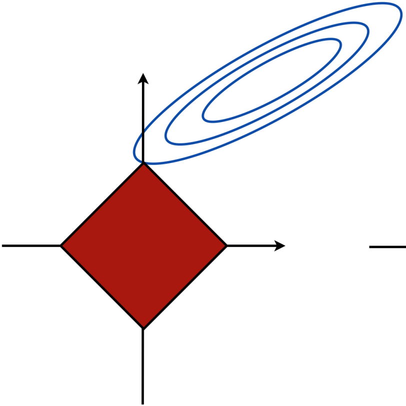
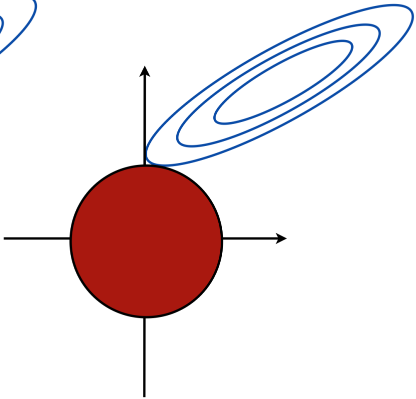


L1 regularization



L2 regularization

- Advantages
  - strong theoretical guarantees
  - sparse solution
  - feature selection
- Disadvantages
  - no natural use of kernels (next slides!)
  - no closed-form solution (not necessary, but can be convenient for theoretical analysis)
- **Empirical recipe** to provide better prediction performance:
  - First, perform variable selection using LASSO
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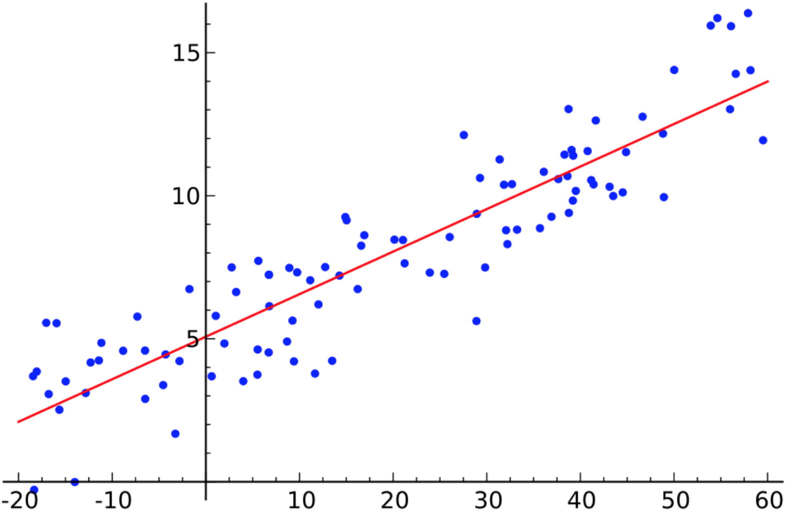
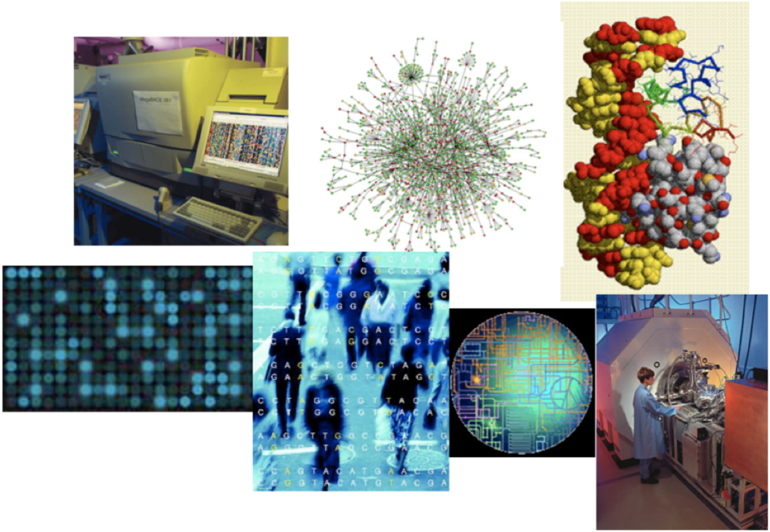
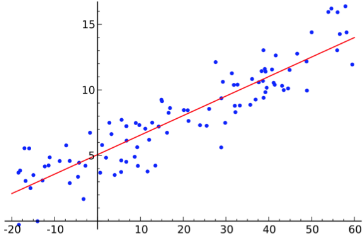
What we know how to solve

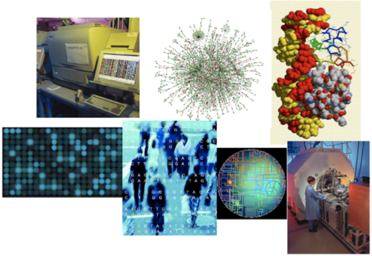


But real data are often more complicated ...



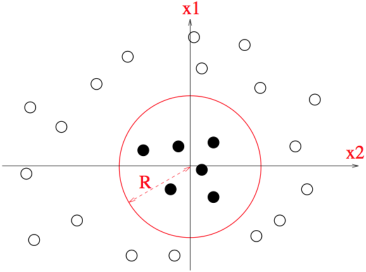
Main goal of using kernels





Show some classical examples how to extend well-understood, linear statistical learning techniques to real-world, complicated, structured, high-dimensional data (texts, time series, graphs, distributions, permutations, ...)

- Efficient computation of inner products in high dimension
- Non-linear decision boundary
- Learning with non-vectorial inputs
- More informative features
- Kernels allow to perform pairwise comparisons



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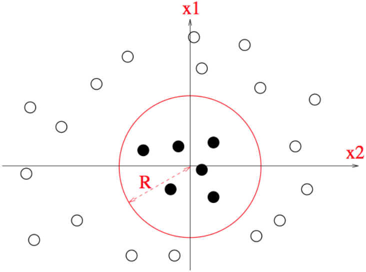
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m



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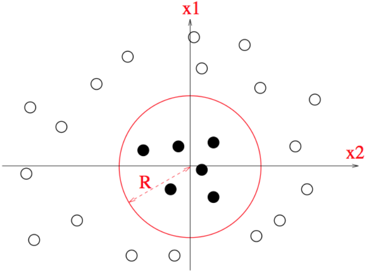

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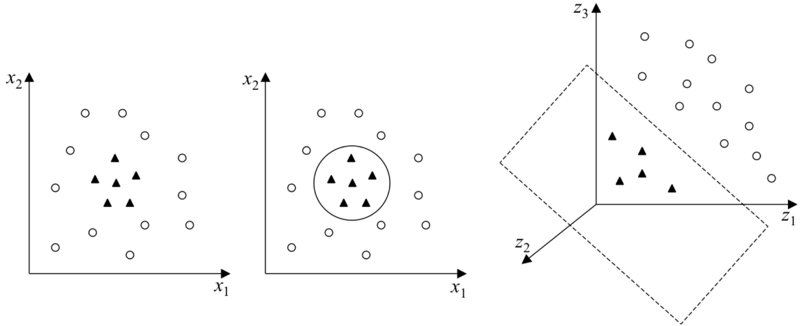
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m



For $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$, let $\Phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$. Then

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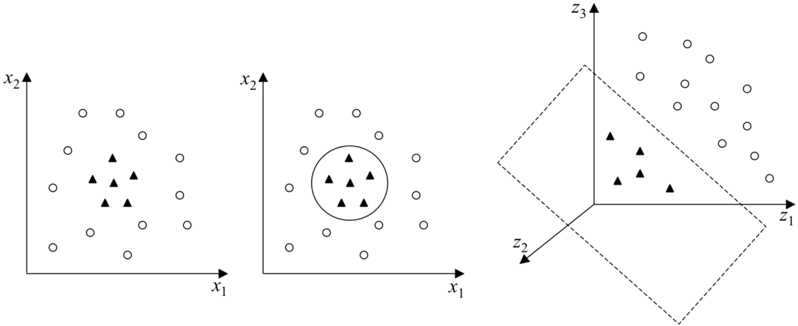

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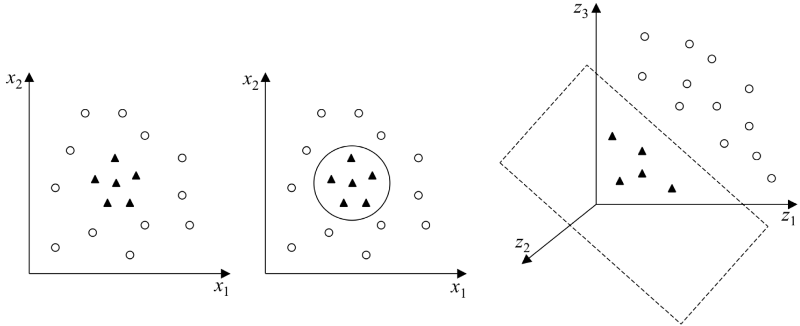
Example: polynomial kernel



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- **Idea**:
  - Define $K : X \times X \to \mathbb{R}$ called kernel, such that

$$\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')^{\top} = K(\mathbf{x}, \mathbf{x}')$$

  - K is often interpreted as a similarity measure

- **Benefits**:
  - Efficiency: K is often more efficient to compute than Φ and the dot product
  - Flexibility: K can be chosen arbitrarily so long as the existence of Φ is guaranteed (PDS condition or Mercer's condition)

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$$\begin{aligned} K(\mathbf{x}, \mathbf{x}') &= (x_1 x_1' + x_2 x_2' + c)^2 \\ &= \left[x_1^2, x_2^2, \sqrt{2} x_1 x_2, \sqrt{2c} x_1, \sqrt{2c} x_2, c\right] \cdot \begin{bmatrix} (x_1')^2 \\ (x_2')^2 \\ \sqrt{2} x_1' x_2' \\ \sqrt{2c} x_1' \\ \sqrt{2c} x_2' \\ c \end{bmatrix} \end{aligned}$$

- **Gaussian kernels**:

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right), \, \sigma \neq 0$$

- **Sigmoid kernels**:

$$K(\mathbf{x}, \mathbf{x}') = \tanh(a(\mathbf{x} \cdot \mathbf{x}') + b), \;\; a, b > 0$$

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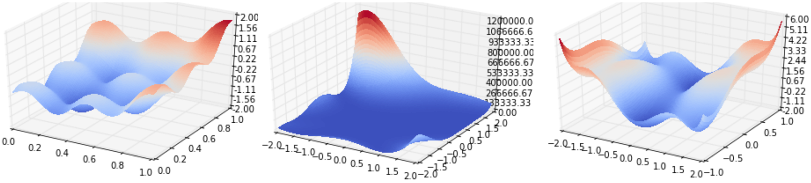

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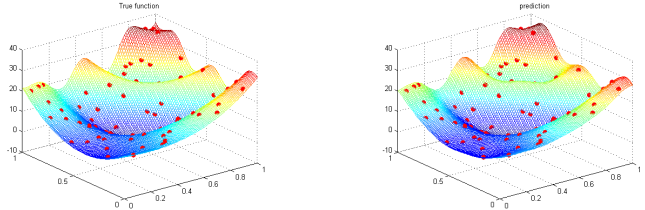

Figure – Mystery function (left) and an approximation (right) for the training sample of size 80

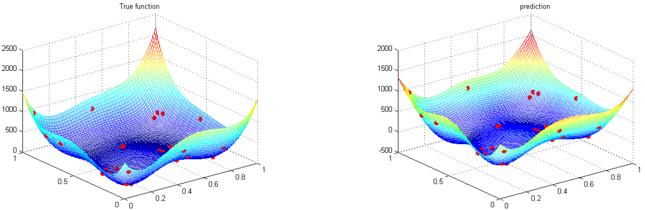

Figure – Himmelblau function (left) and an approximation (right) for the training sample of size 40

- Advantages
  - strong theoretical guarantees
  - generalization to outputs in $\mathbb{R}^p$: single matrix inversion
  - use of kernels
- Disadvantages
  - solution is not sparse
  - training time for large matrices: low-rank approximations of kernel matrix, e.g., Nyström approximation, partial Cholesky decomposition
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- Disadvantages of LASSO:
  - In the $d > m$ case, the lasso selects at most m variables before it saturates, because of the nature of the convex optimization problem. However, e.g. in gene selection problems typically $d > m$
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- If there is a group of variables among which the pairwise correlations are very high, then the LASSO tends to select only one variable from the group and does not care which one is selected
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$$\begin{aligned} \widehat{w}_i(Ridge) &= \widehat{w}_i(OLS)/(1+\lambda_2), \\ \widehat{w}_i(LASSO) &= (|\widehat{w}_i(OLS)| - \lambda_1/2)_+ \cdot \mathrm{sign}(\widehat{w}_i(OLS)), \\ \widehat{w}_i(EN) &= \frac{(|\widehat{w}_i(OLS)| - \lambda_1/2)_+}{1+\lambda_2} \cdot \mathrm{sign}(\widehat{w}_i(OLS)) \end{aligned}$$

where $(x)_+ = \max(x, 0)$

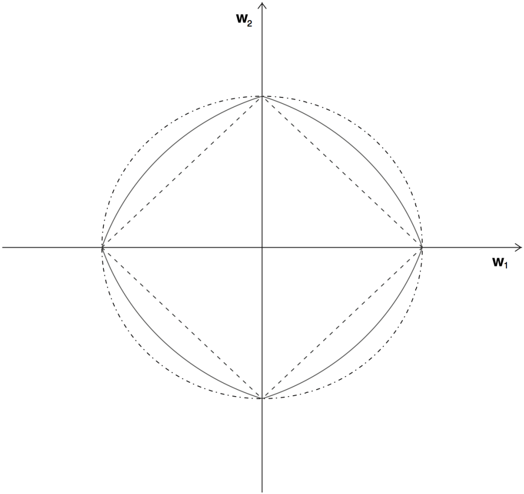

Figure – Two-dimensional contour plots of the penalty ($\cdot - \cdot - \cdot -$, shape of the ridge penalty; $- - -$, contour of the lasso penalty; ——, contour of the elastic net penalty with $\alpha = 0.5$): we see that singularities at the vertices and the edges are strictly convex; the strength of convexity varies with α [Hui Zou, Trevor Hastie]

- It can be proved that in Elastic Net, highly correlated predictors will have similar regression coefficients
- Given data $\{\mathbf{X}, \mathbf{y}\}$ and parameters (λ, α), the response $\mathbf{y}$ is centred and the predictors $\mathbf{X}$ are standardized
- Let $\widehat{\mathbf{w}}(\lambda, \alpha)$ be the elastic net estimate. Suppose that $\widehat{w}_i(\lambda, \alpha)\widehat{w}_j(\lambda, \alpha) > 0$
- Define
$$D_{(\lambda,\alpha)}(i,j) = \frac{1}{\|\mathbf{y}\|_1}|\widehat{w}_i(\lambda, \alpha) - \widehat{w}_j(\lambda, \alpha)|,$$
then
$$D_{(\lambda,\alpha)}(i,j) \leq \frac{1}{\lambda\alpha}\sqrt{\{2(1-\rho)\}},$$
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- Elastic Net produces a sparse model with good prediction accuracy, while encouraging a grouping effect
- Efficient computation algorithm for Elastic Net is derived based on LARS
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