Intro to Regression

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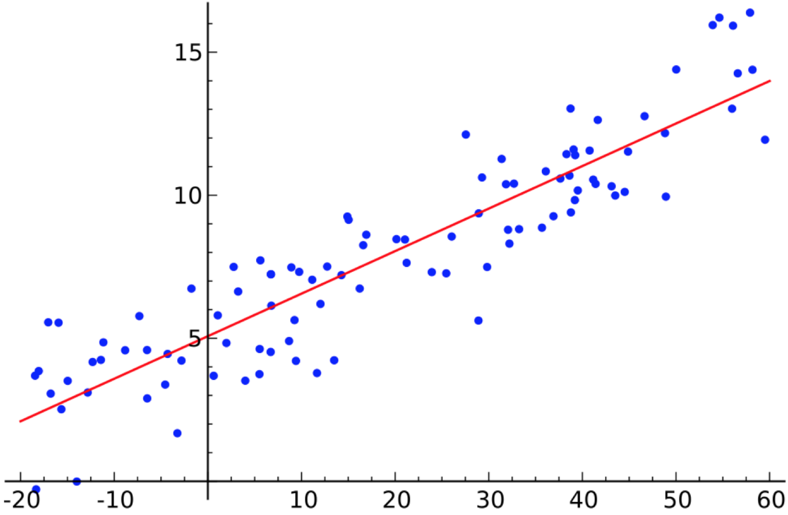
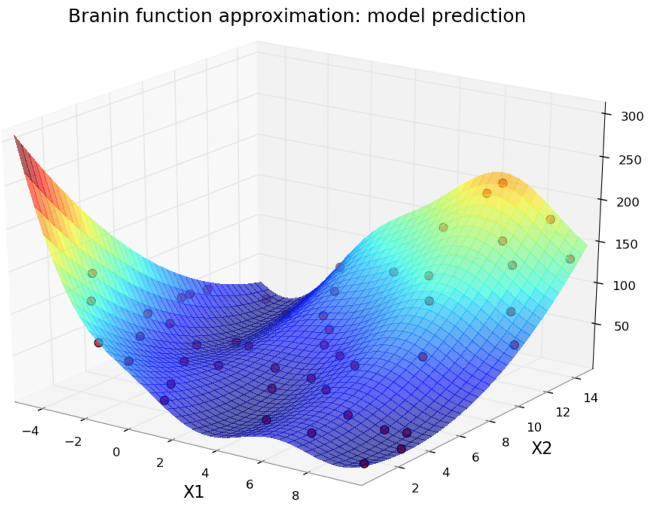
Outline

Regression




Branin function approximation: model prediction
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4
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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

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

Regression Problem Statement

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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:
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Example: Shop revenue prediction

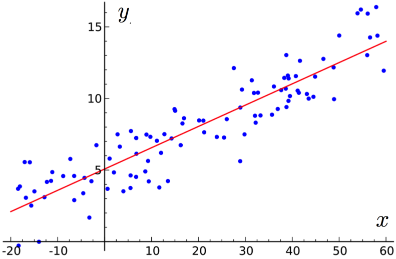
- **Object** $\mathbf{x}$: place to open a new restaurant
- **Label** y: revenue after one year of operation
- **Features**: demographic properties of a considered city district, prices for real estate in a local neighborhood, availability of offices nearby, etc.
- **Challenges**:
  - small sample size
  - 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

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



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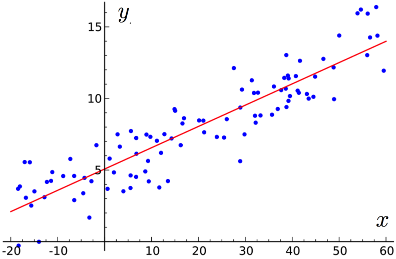

- Rewrite objective function as $F(\mathbf{W}) = \frac{1}{m}\left\|\mathbf{X}\mathbf{W} - \mathbf{Y}\right\|^2$, where

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

- Convex and differentiable function

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$$\nabla F(\mathbf{W}) = \frac{2}{m}\mathbf{X}^\top\left(\mathbf{XW} - \mathbf{Y}\right)$$

Linear Regression: Solution I

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

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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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Ridge Regression: Solution

- Assume $b = 0$: often constant feature is used
- Rewrite objective function as

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

- Convex and differentiable function
- **Solution**:

$$\mathbf{W} = \underbrace{(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}}_{\text{always invertible!}} \mathbf{X}^\top\mathbf{Y}$$

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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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- We can easily prove that

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- With

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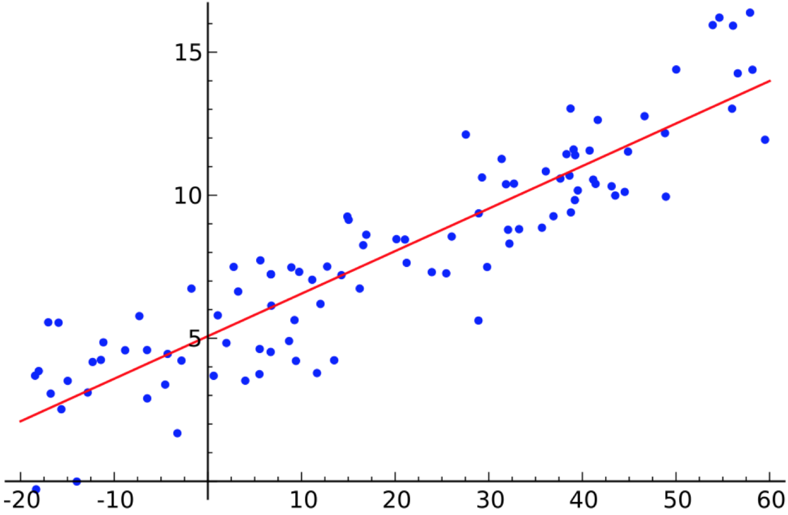
Type	Solution	Prediction
Primal	$O(md^2 + d^3)$	$O(d)$
Dual	$O(\varkappa m^2 + m^3)$	$O(\varkappa m)$

Here $\varkappa$ denotes the time complexity of computing a dot product;
Euclidian dot product $\varkappa = O(d)$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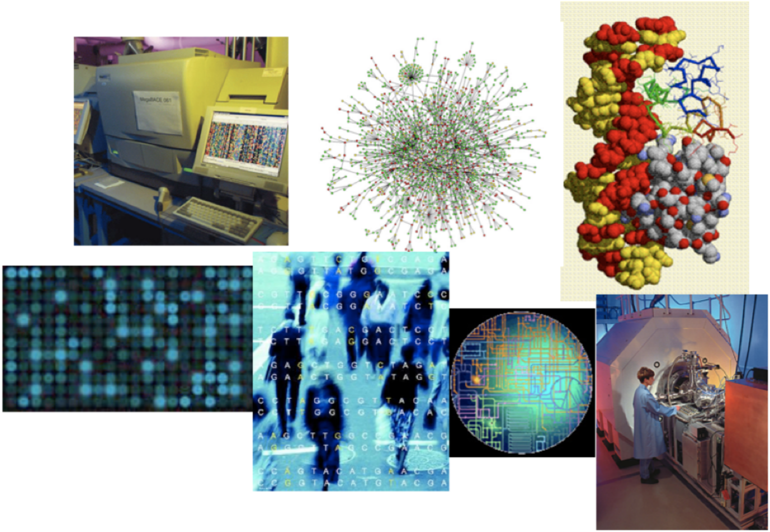
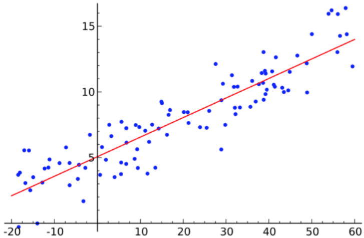
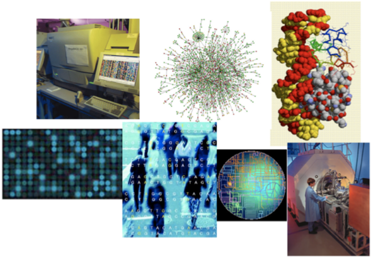
But real data are often more complicated ...



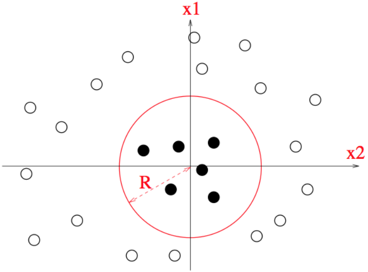
Main goal of using kernels





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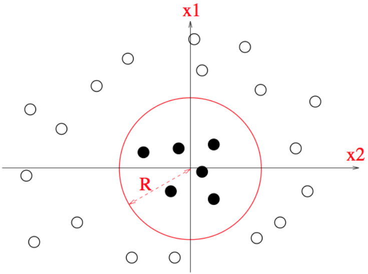
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m



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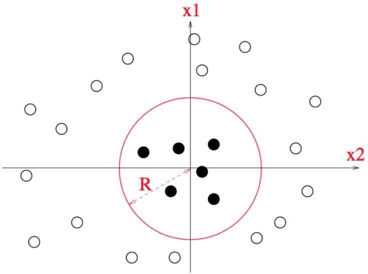

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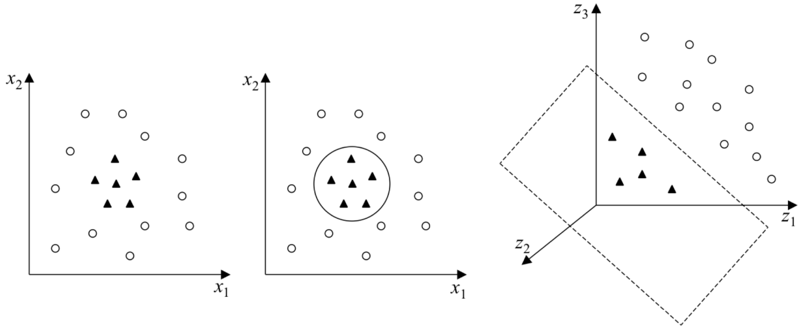
Example: polynomial kernel



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

$$K(\mathbf{x}', \mathbf{x}) = \Phi(\mathbf{x}') \cdot \Phi(\mathbf{x})^\top \quad \text{[dot product of features]}$$

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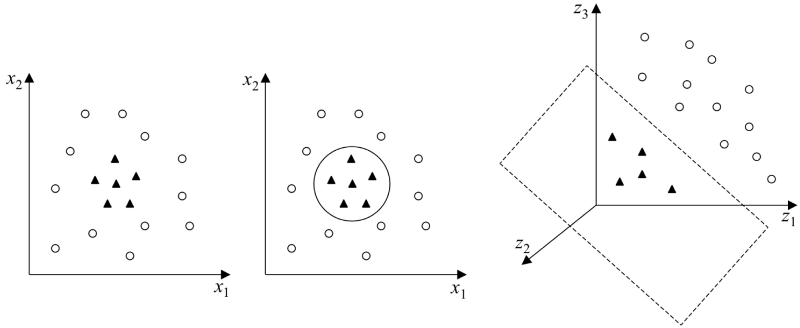

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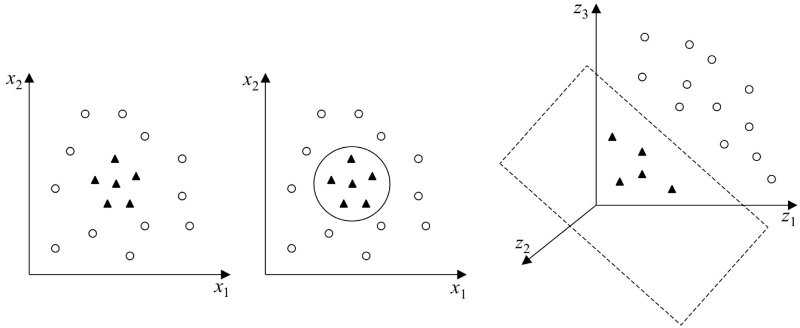
K(\mathbf{x}', \mathbf{x}) &= \Phi(\mathbf{x}') \cdot \Phi(\mathbf{x})^\top \quad \text{[dot product of features]} \\
&= x_1^2 (x_1')^2 + 2 x_1 x_2 x_1' x_2' + x_2^2 (x_2')^2
\end{aligned}
$$



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&= x_1^2(x_1')^2 + 2x_1x_2x_1'x_2' + x_2^2(x_2')^2 \\
&= (x_1x_1' + x_2x_2')^2 = (\mathbf{x}' \cdot \mathbf{x}^\top)^2
\end{aligned}
$$

Kernel Methods

- **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

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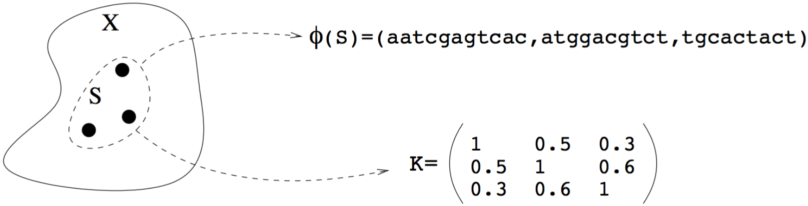
Representation by pairwise comparisons



Idea:

- Define a "comparison function": $K : X \times X \to \mathbb{R}$
- Represent a set of m data points $S = \{\mathbf{x}_1, \dots, \mathbf{x}_m\}$ by the $m \times m$ matrix
$$[K]_{i,j} := K(\mathbf{x}_i, \mathbf{x}_j)$$

Example: polynomial kernels

- **Definition**:

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d,\ K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}' \cdot \mathbf{x}^\top + c)^p,\ c > 0$$

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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**:

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

- **Definition**: a kernel $K : X \times X \to \mathbb{R}$ is *positive definite symmetric* (PDS) is for any $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subseteq X$ the matrix $\mathrm{K} = [K(\mathbf{x}_i, \mathbf{x}_j)]_{ij} \in \mathbb{R}^{m \times m}$ is symmetric positive semi-definite (SPSD)

- Matrix K SPSD if symmetric and one of the 2 equiv. cond.'s:
  - its eigenvalues are non-negative
  - for any $\mathbf{c} \in \mathbb{R}^{m \times 1}$, $\mathbf{c}^\top \mathrm{K} \mathbf{c} = \sum_{i,j=1}^{m} c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0$

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Finite-dimensional representation

- Usual linear ridge regression in dual representation

$$\widehat{f}(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i (\mathbf{x} \cdot \mathbf{x}_i^\top)$$

with

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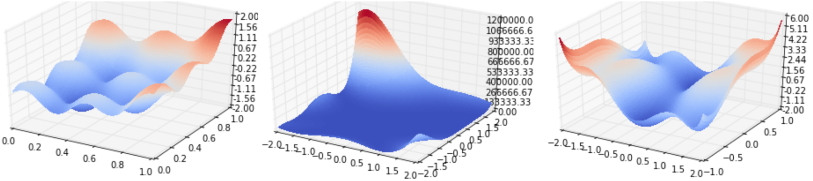

Example: Kernel ridge regression (II)

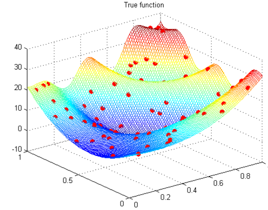

Figure – Mystery function (left) and an approximation (right) for the training sample of size 80

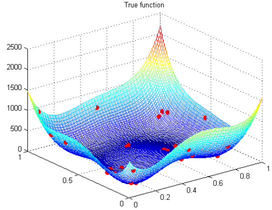

Figure – Himmelblau function (left) and an approximation (right) for the training sample of size 40

Comments

- Advantages
  - strong theoretical guarantees
  - generalization to outputs in $\mathbb{R}^p$: single matrix inversion
  - use of kernels
- Disadvantages
  - solution is not sparse
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- **Optimization problem**: "Least Absolute Shrinkage and Selection Operator"

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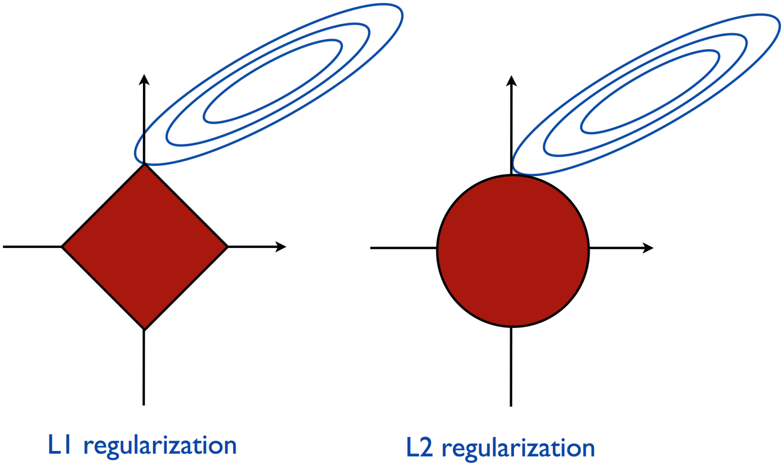
Sparsity of L_1 regularization



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  - sparse solution
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  - no closed-form solution (not necessary, but can be convenient for theoretical analysis)
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- **Prediction accuracy** and **model interpretation** are two important aspects of regression models
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- LASSO does shrinkage and variable selection simultaneously for better prediction and model interpretation
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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
- It has been empirically observed that the prediction performance of the LASSO is dominated by ridge regression
- **Elastic Net**: Regression, variable selection, with the capacity of selecting groups of correlated variables.
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Motivation for Elastic Net II

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- **Elastic Net** combines l_1 and l_2 penalties
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- It can be proved that in case of orthogonal design matrix ($\mathbf{X}^\top \mathbf{X} = \mathrm{I}$) analytical solution exists

Naive Elastic Net

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$$\begin{aligned}\widehat{w}_i(Ridge) &= \widehat{w}_i(OLS)/(1+\lambda_2),\\ \widehat{w}_i(LASSO) &= \left(|\widehat{w}_i(OLS)| - \lambda_1/2\right)_+ \cdot \mathrm{sign}(\widehat{w}_i(OLS)),\\ \widehat{w}_i(EN) &= \frac{\left(|\widehat{w}_i(OLS)| - \lambda_1/2\right)_+}{1+\lambda_2} \cdot \mathrm{sign}(\widehat{w}_i(OLS))\end{aligned}$$

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

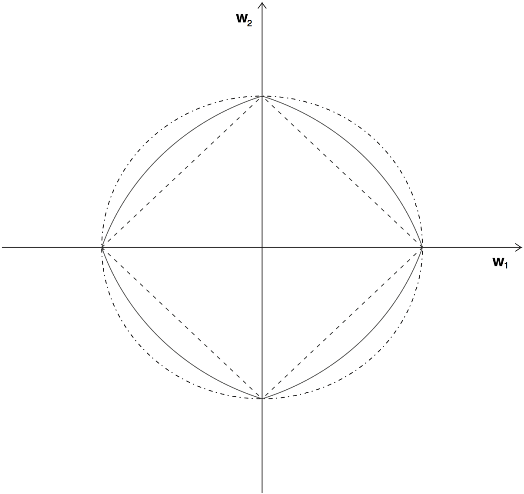

Figure – Two-dimensional contour plots of the penalty ($\cdot - \cdot - \cdot -$, shape of the ridge penalty; $- - -$, contour of the lasso penalty; ——, contour of the elastic net penalty with $\alpha = 0.5$): we see that singularities at the vertices and the edges are strictly convex; the strength of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

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- Let $\widehat{\mathbf{w}}(\lambda, \alpha)$ be the elastic net estimate. Suppose that $\widehat{w}_i(\lambda, \alpha)\widehat{w}_j(\lambda, \alpha) > 0$
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- Efficient computation algorithm for Elastic Net is derived based on LARS
- Empirical results and simulations demonstrate its superiority over LASSO (LASSO can be viewed as a special case of Elastic Net)
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