Intro to Regression

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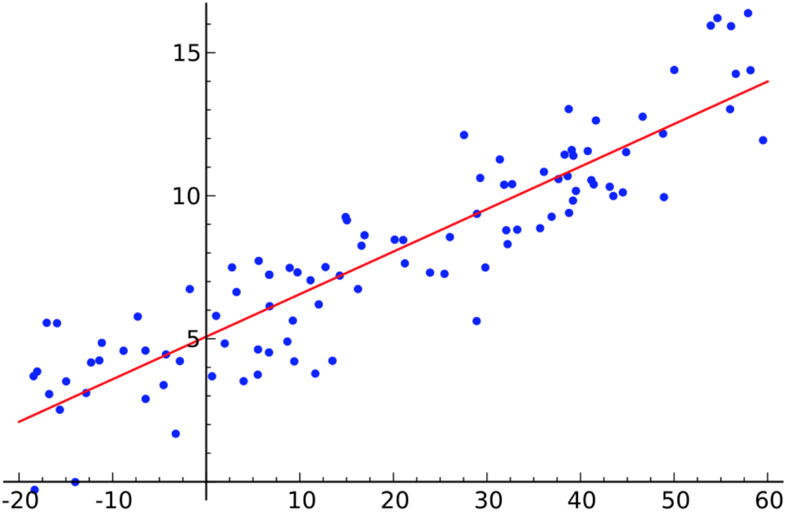
Outline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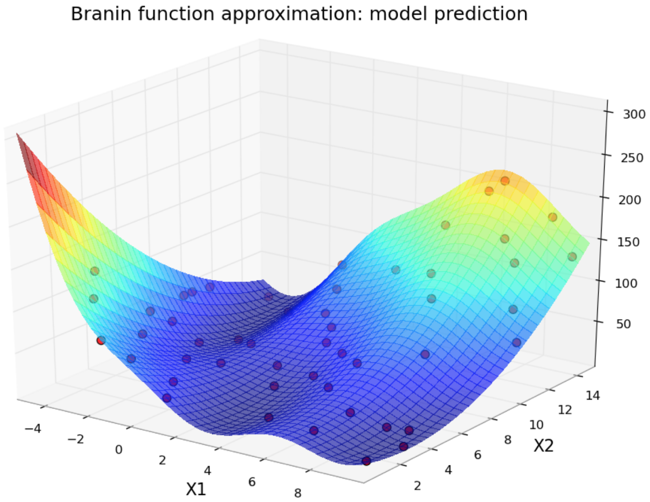
Branin function approximation: model prediction
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X2

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

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  - $Y = \mathbb{R}$ or $Y = [-M, M]$ for some $M > 0$
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Regression Problem

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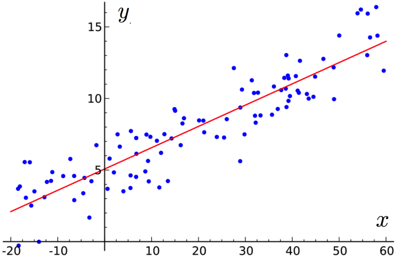
- **Object** $\mathbf{x}$: place to open a new restaurant
- **Label** y: revenue after one year of operation
- **Features**: demographic properties of a considered city district, prices for real estate in a local neighborhood, availability of offices nearby, etc.
- **Challenges**:
  - — small sample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

- Hypothesis set: linear functions

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

- **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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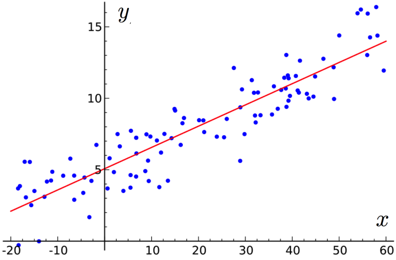

- Rewrite objective function as $F(\mathbf{W}) = \frac{1}{m}\|\mathbf{X}\mathbf{W} - \mathbf{Y}\|^2$, where

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

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

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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- With
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Direct Dual Solution: another representation

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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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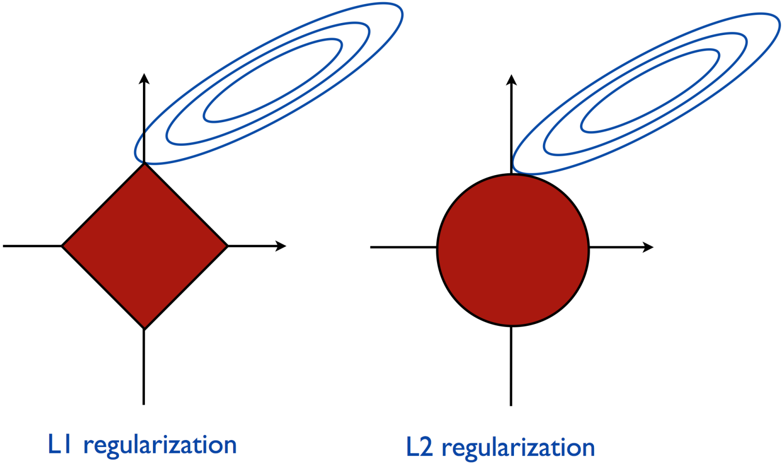
Sparsity of L_1 regularization



- 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:
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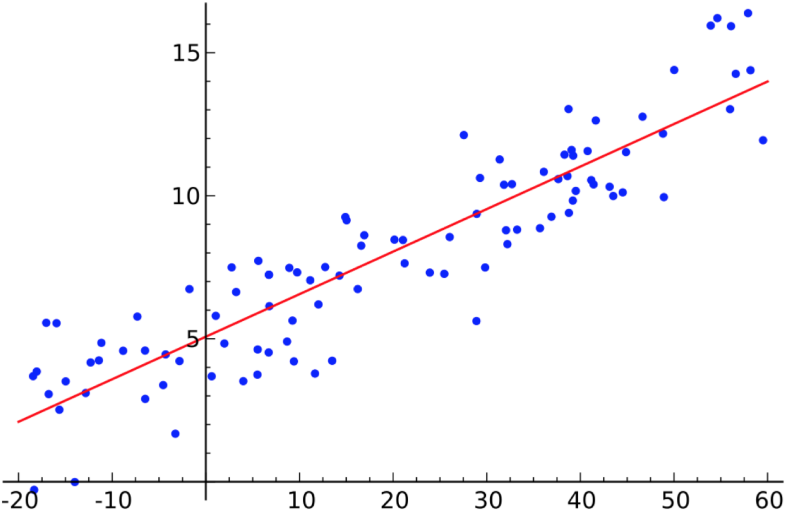
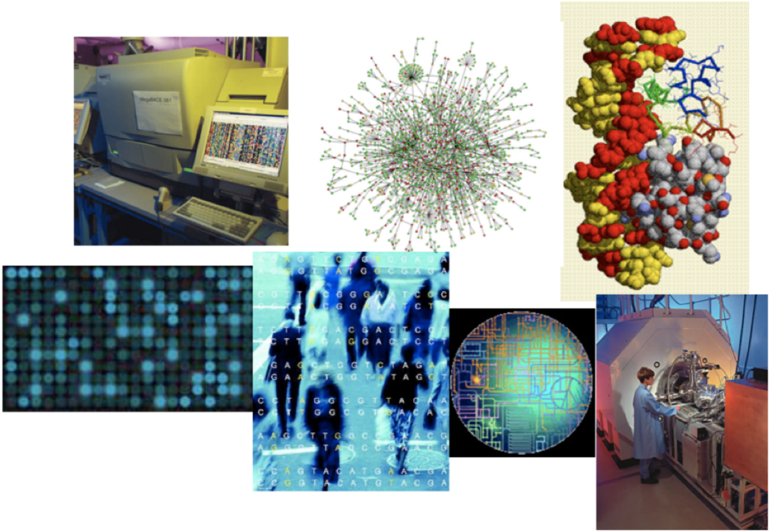
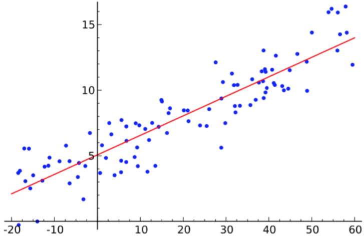
What we know how to solve

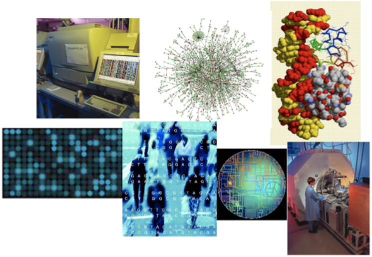


But real data are often more complicated ...



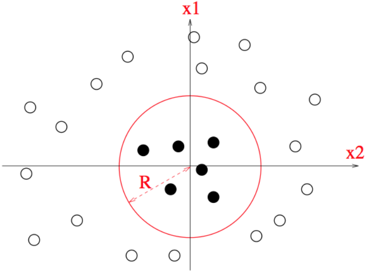
Main goal of using kernels





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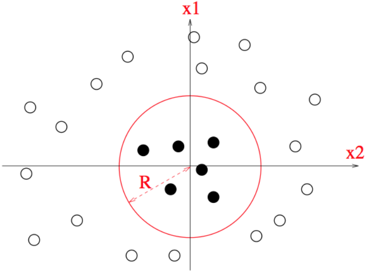
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m



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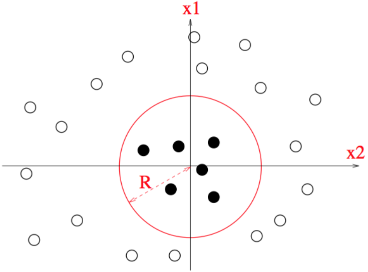

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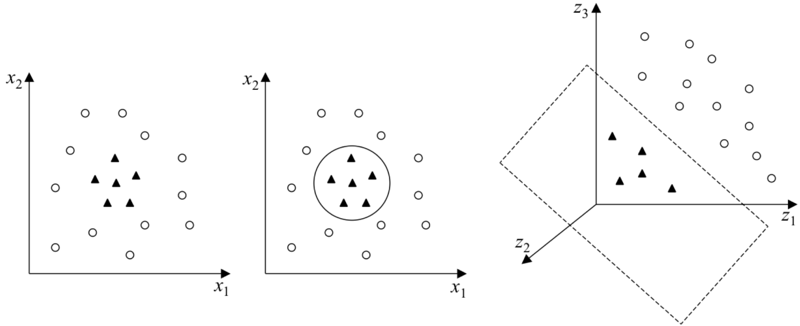
Example: polynomial kernel



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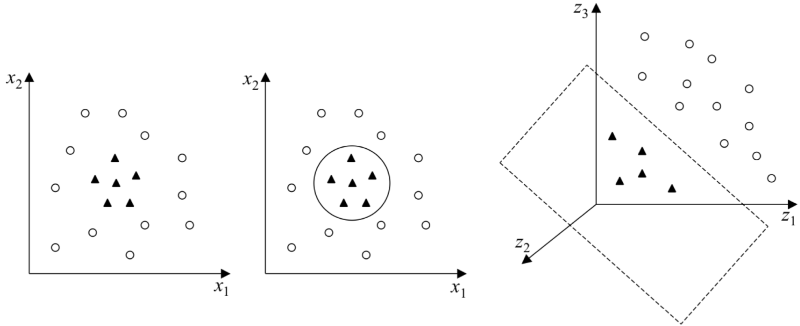

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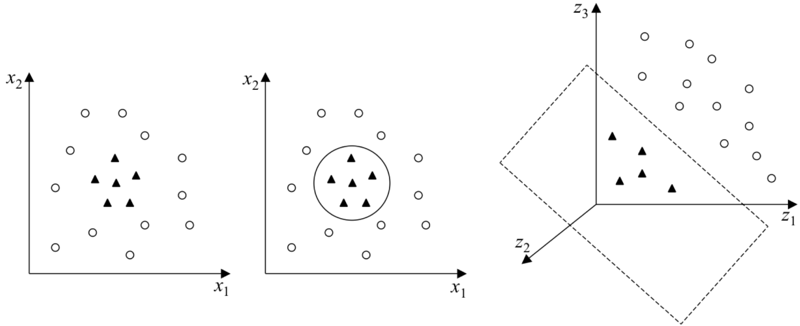

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- **Idea**:
  - Define $K : X \times X \to \mathbb{R}$ called kernel, such that
  $$\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')^\top = K(\mathbf{x}, \mathbf{x}')$$
  - K is often interpreted as a similarity measure

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- **Gaussian kernels**:

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

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

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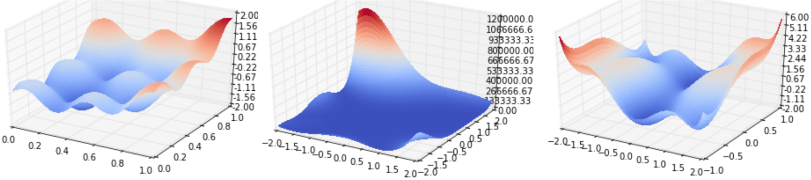

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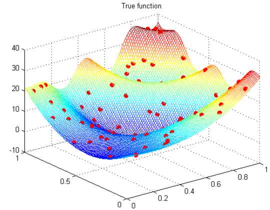

Figure – Mystery function (left) and an approximation (right) for the training sample of size 80

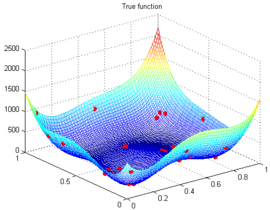

Figure – Himmelblau function (left) and an approximation (right) for the training sample of size 40

- 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:
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\end{aligned}$$

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

Comparison of Penalties

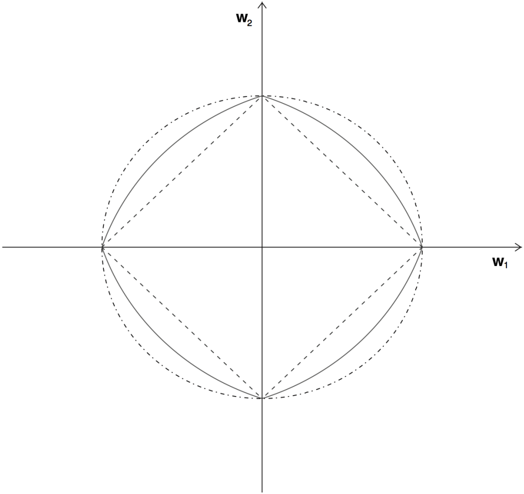

Figure – Two-dimensional contour plots of the penalty ($\cdot - \cdot - \cdot -$, shape of the ridge penalty; $- - -$, contour of the lasso penalty; ——, contour of the elastic net penalty with $\alpha = 0.5$): we see that singularities at the vertices and the edges are strictly convex; the strength of 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
$$D_{(\lambda,\alpha)}(i,j) \leq \frac{1}{\lambda\alpha}\sqrt{\{2(1-\rho)\}},$$
where ρ is the sample correlation between the i-th and j-th columns of the matrix $\mathbf{X}$
- This theorem provides a quantitative description for the grouping effect of Elastic Net

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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
- Empirical results and simulations demonstrate its superiority over LASSO (LASSO can be viewed as a special case of Elastic Net)
- For Elastic Net, two parameters should be tuned/selected on training and validation data set. For LASSO, there is only one tuning parameter
- Although Elastic Net is proposed with the regression model, it can also be extend to classification problems (such as gene selection)

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