Business Analytics

1. Prediction, 1.3 Regularized Loss Models

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Outline

1. Overfitting and Regularization
2. Prediction Functions
3. Sparse Predictors
4. Learning Algorithms

Outline

Overall Procedure

1. define a **prediction function** $\hat{y}$ that depends on some **model parameters** $\Theta \in \mathbb{R}^q$, e.g., for regression, a linear model:

$$\hat{y}(x;\Theta) := \beta_0 + \beta^T x = \beta_0 + \sum_{i=1}^{p} \beta_i x_i, \quad \Theta := (\beta_0, \beta_1, \ldots, \beta_p)$$

2. the **training error**

$$\ell(\Theta; \mathcal{D}^{\text{train}}) := \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{(x,y)\in\mathcal{D}^{\text{train}}} \ell(y, \hat{y}(x;\Theta))$$

is called **objective function**

$$f(\Theta; \mathcal{D}^{\text{train}}) := \ell(\Theta; \mathcal{D}^{\text{train}})$$

3. find the parameters Θ^* that **minimize the objective function** numerically.

Overall Procedure

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2. define a **regularization function**

$$R : \mathbb{R}^q \to \mathbb{R}_0^+, \quad \text{e.g., } R(\Theta) := ||\Theta||^2 = \sum_{i=1}^{q} \Theta_i^2$$

that penalizes complex models. Its combination with the **training error**

$$\ell(\Theta; \mathcal{D}^{\text{train}}) := \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{(x,y) \in \mathcal{D}^{\text{train}}} \ell(y, \hat{y}(x; \Theta))$$

is called **objective function**

$$f(\Theta; \mathcal{D}^{\text{train}}) := \ell(\Theta; \mathcal{D}^{\text{train}}) + \lambda R(\Theta), \quad \lambda \in \mathbb{R}_0^+$$

3. find the parameters Θ^* that **minimize the objective function**

Overfitting

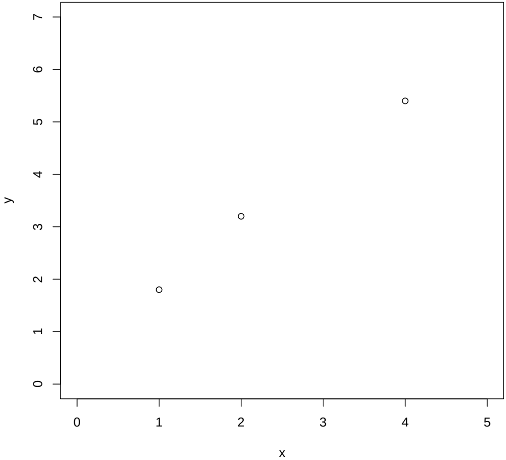
Example:
Assume the true data generating process is

$$Y = 1 + X_1 + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 0.1)$$

and we draw the following sample

x_1	y
1.0	1.8
2.0	3.2
4.0	5.4

Overfitting



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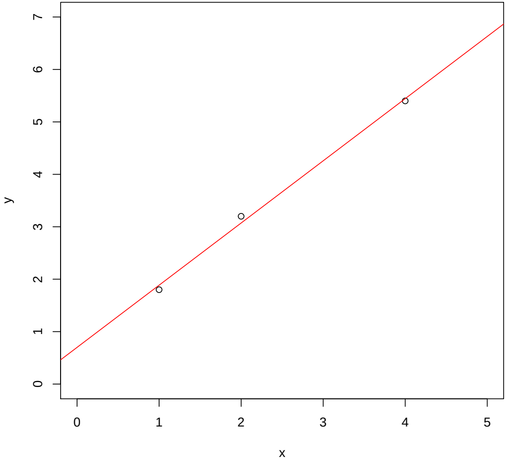

The linear model with minimal training error is model #1:

$$\hat{y}(x_1) := 0.7 + 1.186\, x_1, \quad \mathrm{RMSE}(\hat{y}) = 0.093$$

Overfitting

Now lets assume we measure 3 further variables x_2, x_3 and x_4, not correlated with the target Y at all (**noise**):

x_1	x_2	x_3	x_4	y
1.0	1.0	0.0	0.0	1.8
2.0	0.0	1.0	0.0	3.2
4.0	0.0	0.0	1.0	5.4

Now, a linear model with minimal training error is model #2:

$$\hat{y}(x_1) := 0.7 + 1.186\,x_1 - 0.086\,x_2 + 0.128\,x_3 - 0.044\,x_4, \quad \text{RMSE}(\hat{y}) = 0$$

And another one is model #3:

$$\hat{y}(x_1) := 0.0 + 0.0\,x_1 + 1.8\,x_2 + 3.2\,x_3 + 5.4\,x_4, \quad \text{RMSE}(\hat{y}) = 0$$

These models **fit noise** or **overfit**.

Overfitting

How to **avoid overfitting**?

- do not include noisy variables

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- employ model selection to find out which variables are noisy (**variable selection**)
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- force all parameters to be small (**shrinking**)

Why Small Parameters Prevent Overfitting

Assume we force all parameters β_i to be $|\beta_i| \leq 2$.
Then model #3 is no longer allowed:

$$\hat{y}(x_1) := 0.0 + 0.0\,x_1 + 1.8\,x_2 + 3.2\,x_3 + 5.4\,x_4, \quad \text{RMSE}(\hat{y}) = 0$$

Model #4 is already much better:

$$\hat{y}(x_1) := 2.0 + 0.35\,x_1 - 0.55\,x_2 + 0.5\,x_3 + 2.0\,x_4, \quad \text{RMSE}(\hat{y}) = 0$$

Assume we force all parameters β_i to have $\sum_{i=0}^{p} |\beta_i| \leq 3$.
Model #5 is again much better:

$$\hat{y}(x_1) := 0.5 + 1.125\,x_1 - 0.175\,x_2 - 0.45\,x_3 + 0.4\,x_4, \quad \text{RMSE}(\hat{y}) = 0$$

Outline

Linear Model

$$\hat{y}(x) := \beta_0 + \beta^T x = \beta_0 + \sum_{i=1}^{p} \beta_i x_i$$

Polynomial Model

of degree 2:

$$\hat{y}(x) := \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i=1}^{p} \sum_{j=i}^{p} \beta_{i,j} x_i x_j$$

e.g.,

$$\hat{y}(x_1, x_2) := \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{1,1} x_1^2 + \beta_{2,2} x_2^2 + \beta_{1,2} x_1 x_2$$

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of degree 3:

$$\hat{y}(x) := \beta_0 + \sum_{i=1}^{p} \beta_i x_i + \sum_{i=1}^{p} \sum_{j=1}^{p} \beta_{i,j} x_i x_j + \sum_{i=1}^{p} \sum_{j=i}^{p} \sum_{k=j}^{p} \beta_{i,j,k} x_i x_j x_k$$

e.g.,

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of degree d:

$$\hat{y}(x) := \sum_{J \in \Delta_{p,d}} \beta_J x^J \qquad \text{where } x^J := \prod_{i=1}^{p} x_i^{J_i}, \quad J \in \Delta_{p,d}$$

$$\Delta_{p,d} := \{J \in \mathbb{N}^p \mid \sum_{i=1}^{p} J_i \leq d\}$$

Factorized Polynomial Models

of degree d:

$$\hat{y}(x) := \sum_{J \in \Delta_{p,d}} \beta_J x^J$$

with

$$\beta_J := \sum_{k=1}^{K} \phi_k^J, \quad \phi_k \in \mathbb{R}^p$$

Kernels

$$\hat{y}(x) := \beta_0 + \sum_{i=1}^{N} \alpha_i y_i k(x_i, x), \quad \text{with } (x_1, y_1), \ldots, (x_N, y_N) \in \mathcal{D}^{\text{tra}}$$

and a **kernel** $k : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}_0^+$, e.g.,

polynomial kernel

$$k(x, x') := (1 + x^T x')^d, \quad d \in \mathbb{N} \text{ degree}$$

radial basis function kernel

$$k(x, x') := e^{\gamma x^T x'}, \quad \gamma \in \mathbb{R}^+$$

Models — Many Fancy Names

prediction function	loss	regularization	model name
linear	L2	—	regression, least squares
linear	L2	L2	ridge regression
kernel	L2	—	kernel regression
linear	L2	L1	lasso
linear	L2	L1+L2	elastic net
linear/kernel	ϵ-insensitive	L2	support vector regression
⋮	⋮	⋮	⋮
linear	hinge	—	perceptron
linear/kernel	hinge	L2	support vector machine
linear/kernel	squared hinge	L2	L2 support vector machine
logistic(linear)	loglikelihood	—	logistic regression
logistic(linear)	loglikelihood	L2	logistic ridge regression
⋮	⋮	⋮	⋮

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Sparse predictors

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- the products a customer bought in an online shop.
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Sparse predictors

- can be **stored more compact** in $O(p_{\text{nz}}) < O(p)$ by storing only indices and values of non-zero components:

$$x = (5, 0, 0, 3, 4, 0, 0, 0, 0, 0) \in \mathbb{R}^{10} \leftrightarrow x = ((1, 5), (4, 3), (5, 4)) \in (\mathbb{N}\times\mathbb{R}$$

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- can be **multiplied faster** with a dense or sparse vector in $O(p_{\text{nz}}) < O(p)$:

  $$\beta^T x = \sum_{i=1}^{p} \beta_i x_i \leftrightarrow \beta^T x = \sum_{i=1}^{|x|} \beta_{x_{i,1}} x_{i,2}$$

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Objective Function

Learning a model means to find the parameters $\hat{\theta}$ with a **minimum of the objective function** f:

$$\hat{\Theta} := \arg\min_{\Theta} f(\Theta) := \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{(x,y)\in\mathcal{D}^{\text{train}}} \ell(y, \hat{y}(x;\Theta)) + \lambda R(\Theta)$$

with $\lambda \in \mathbb{R}_0^+$ fixed.

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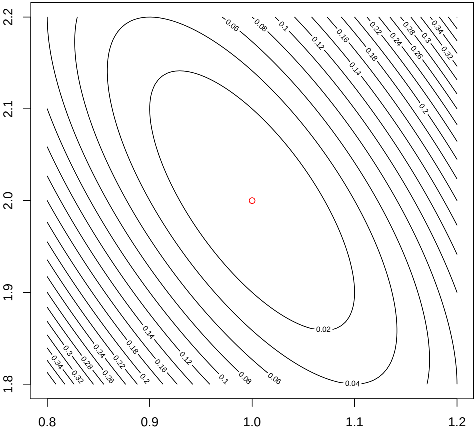
with $\lambda \in \mathbb{R}_0^+$ fixed.

- only for regression and ridge regression this is an unconstrained quadratic problem that easily can be solved as a system of linear equations

$$(X^T X + \lambda I)\hat{\beta} = X^T y$$

- in all other cases a solution needs to be found numerically.

Objective Function



$$\hat{\Theta} := \arg\min_{\Theta} f(\Theta) := \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{(x,y)\in\mathcal{D}^{\text{train}}} \ell(y, \hat{y}(x;\Theta)) + \lambda R(\Theta)$$

Gradient Descent

$$\text{choose } \Theta^{(0)} \in \mathbb{R}^p$$

$$\Theta^{(t+1)} := \Theta^{(t)} - \eta^{(t)} \frac{\partial f}{\partial \Theta}(\Theta^{(t)}), \quad t = 0, 1, 2, \ldots$$

$$\text{stop once } ||\frac{\partial f}{\partial \Theta}(\Theta^{(t)})|| < \epsilon$$

with

- $\eta^{(t)} \in \mathbb{R}^+$ called **step size** / **learning rate**.
- $\epsilon \in \mathbb{R}^+$ called **minimum gradient norm** / **stopping criterion**.

Gradient Descent

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$$
\frac{\partial f}{\partial \Theta}(\Theta) = \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{(x,y) \in \mathcal{D}^{\text{train}}} \frac{\partial \ell}{\partial \hat{y}}(y, \hat{y}(x; \Theta)) \frac{\partial \hat{y}}{\partial \Theta}(x; \Theta) + \lambda \frac{\partial R}{\partial \Theta}(\Theta)
$$

Gradient Descent

Example: logistic regression.

$$\ell(y,\hat{y}) = -y \log \hat{y} - (1-y)\log(1-\hat{y})$$

$$\frac{\partial \ell}{\partial \hat{y}}(y,\hat{y}) = -y\frac{1}{\hat{y}} - (1-y)\frac{-1}{1-\hat{y}} = \frac{\hat{y}-y}{\hat{y}\,(1-\hat{y})}$$

$$\hat{y}(x;\Theta) = \text{logistic}(\Theta^T x)$$

$$\frac{\partial \hat{y}}{\partial \Theta_j}(x;\Theta) = \text{logistic}(\Theta^T x) \cdot (1-\text{logistic}(\Theta^T x))x_j$$

$$R(\Theta) = \Theta^T\Theta$$

$$\frac{\partial R}{\partial \Theta_j}(\Theta) = 2\Theta_j$$

$$\rightsquigarrow \quad \frac{\partial f}{\partial \Theta}(\Theta) = \frac{1}{|\mathcal{D}^{\text{train}}|}\sum_{(x,y)\in\mathcal{D}^{\text{train}}}(\hat{y}(x;\Theta)-y)x + 2\lambda\Theta$$

Newton Algorithm

$$\text{choose } \Theta^{(0)} \in \mathbb{R}^p$$

$$\text{solve } \left(\frac{\partial^2 f}{\partial \Theta^2}(\Theta^{(t)})\right) d^{(t)} = -\frac{\partial f}{\partial \Theta}(\Theta^{(t)})$$

$$\Theta^{(t+1)} := \Theta^{(t)} - \eta^{(t)} d^{(t)}$$

$$\text{stop once } ||d^{(t)}|| < \epsilon$$

with

- $\eta^{(t)} \in \mathbb{R}^+$ called **step size** / **learning rate**.
- $\epsilon \in \mathbb{R}^+$ called **minimum gradient norm** / **stopping criterion**.

Stochastic Gradient Descent

Rewrite the objective as a big sum:

$$f(\Theta) = \sum_{i=1}^{n} f_i(\Theta),$$

$$f_i(\Theta) := \ell(y_i, \hat{y}(x_i; \Theta) + \frac{\lambda}{n} R(\Theta)$$

then minimize a summand at a time:

choose $\Theta^{(0)} \in \mathbb{R}^p$

pick uniformly at random $i^{(t)} \in \{1, \ldots, n\}$

$$\Theta^{(t+1)} := \Theta^{(t)} - \eta^{(t)} \frac{\partial f_{i^{(t)}}}{\partial \Theta}(\Theta^{(t)}), \quad t = 0, 1, 2, \ldots$$

stop once $||\Theta^{(t)} - \Theta^{(t-t_0)}|| < \epsilon$

Stochastic Gradient Descent

- Stochastic Gradient Descent (SGD) is as simple to derive and implement as full gradient descent.
- SGD **often converges much faster** than full gradient descent as parameters are updated more quickly.
- For stopping, lack of progress on several iterations (t_0) has to be observed.
- Often the regularization term is not spread uniformaly over all summand functions, but in a clever way s.t. f_i depends on as few Θ_j as possible (**sparse parameter updates**).