Applied Data Science fall 2017

Session 9: Bayesian inference. Linear regression revisited. Regularization - Ridge and Lasso

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Probability: Frequentist vs Bayesian

• Frequentist: P(E) is a frequency of E

 Bayesian: probability P(E) is our degree of confidence that an event E will happen

$$P(C=heads)=0.5$$



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Limitations of frequentist thinking

- Lack of actual observations
- Lack of scalable framework incorporating beliefs and observations
- Non-intuitive interpretation of inference and hypothesis testing

Bayesian thinking

Being certain about uncertainty

"I can live with doubt and uncertainty... I have approximate answers and possible beliefs and different degrees of certainty about different things, and I'm not absolutely sure of anything..."

Richard Feynman

"Now Bayesian statistics are rippling through everything from physics to cancer research, ecology to psychology. Enthusiasts say they are allowing scientists to solve problems that would have been considered impossible just 20 years ago. And lately, they have been thrust into an intense debate over the reliability of research results."

"The essence of the frequentist technique is to apply probability to data. If you suspect your friend has a weighted funfairly coin, for example, and you observe that it came up heads nine times out of 10, a frequentist would calculate

[unfair] coin, for example, and you observe that it came up heads nine times out of 10, a frequentist would calculate the probability of getting such a result with an unweighted [fair] coin. The answer (about 1 percent) is not a direct measure of the probability that the coin is weighted [unfair]; it's a measure of how improbable the nine-in-10 result is — a piece of information that can be useful in investigating your suspicion."

"By contrast, Bayesian calculations go straight for the probability of the hypothesis, factoring in not just the data from the coin-toss experiment but any other relevant information — including whether you have previously seen your friend use a weighted [unfair] coin."

The New York Times, Sept. 29, 2014.

http://www.nytimes.com/2014/09/30/science/the-odds-continually-updated.html

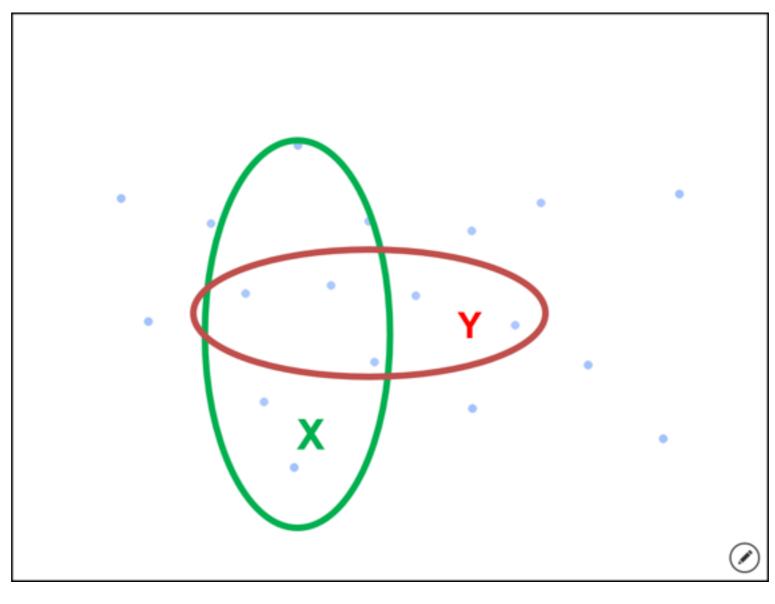


Demand

- Wide-spread of data analysis, statistics
- Variety of problems- intuitive unified framework
- Sufficient computation power



Conditional probability



P(X|Y)

$$P(X \cap Y) = P(X|Y)P(Y)$$



Conditional probability - Bayes theorem

$$P(X \cap Y) = P(X|Y)P(Y)$$

$$P(X \cap Y) = P(Y|X)P(X)$$

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

The core - Bayes theorem

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

Thomas Bayes 1740s Initial Belief + New Data -> Improved Belief

Pierre Simon Laplace 1774. the probability of a cause (given an event) is proportional to the probability of the event

1891, the Scottish mathematician George Chrystal urged: "[Laplace's principle] being dead" - declining subjectivity

Captain Dreyfus used it to demonstrate his innocence

Alan Turing used it to decode the German Enigma cipher



Example

Total of 60% of students were preparing for midterm 40% of those preparing got "A"

Only 15% of those not preparing got "A"

- a) Consider random student. What is your confidence student was preparing? P(prep)=60%
- b) If now you learned the selected student got "A". How does it affect your confidence?

$$P(prep|A) = P(A|prep)P(prep)/P(A) = 0.4x0.6/P(A)$$

$$P(!prep|A) = P(A|!prep)P(!prep)/P(A) = 0.15x0.4/P(A)$$

 $P(prep|A) = 0.24/(0.24+0.06) = 4/5 = 80\%$



Conceptual scheme

1. Express prior beliefs about the unknown parameters

of interest

2. Collect data and evaluate its likelihood with respect

to prior beliefs

$$P(A|prep)=40\%$$

3. Update your beliefs - posterior

P(prep|A)~P(A|prep)P(prep)

posterior~likelihood X prior



Prior beliefs

Important to consider once they exist

But where to get them?

- Theoretical understanding of the subject
- Previous observations
- Guess
- Possibility to model lack of knowledge

Bayesian inference - formalizm

$$y \sim f(\alpha)$$
 $y \sim f(x, \alpha)$

$$D = \{(y_i, x_i), i = 1..N\}$$

discrete

$$P(\alpha|D) = \frac{P(D|\alpha)P(\alpha)}{P(D)} \qquad p(\alpha|D) = \frac{p(D|\alpha)p(\alpha)}{p(D)}$$

$$p(\alpha|D) = \frac{p(D|\alpha)p(\alpha)}{p(D)}$$

$$P(D) = \sum_{\beta} P(D|\beta)P(\beta) \quad p(D) = \int p(D|\beta)p(\beta)d\beta$$

$$p(D) = \int p(D|\beta)p(\beta)d\beta$$

$$p(\alpha|D) \sim p(D|\alpha)p(\alpha)$$

$$posterior \sim likelihood * prior$$



Tossing a coin

$$P(c=1) = \alpha \qquad P(c=0) = 1 - \alpha$$

$$p(\alpha) - prior\ belief$$

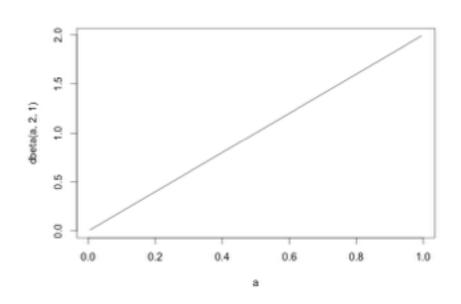
uninformative prior:

$$\alpha \sim Unif(0, 1)$$
 $p(\alpha) = 1$

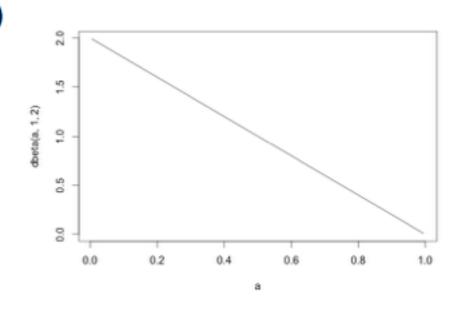


Tossing coin - once

$$p(\alpha|c=1) \sim P(c=1|\alpha)p(\alpha) = \alpha p(\alpha)$$



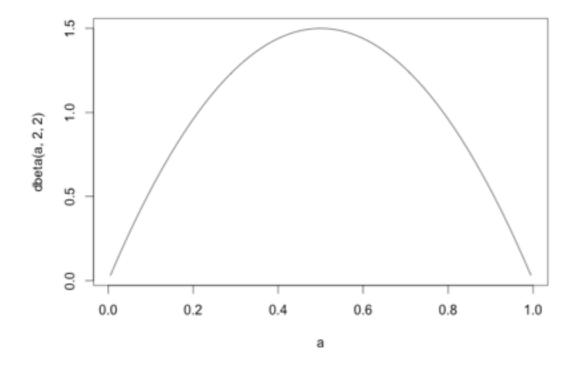
$$p(\alpha|c=0) \sim P(c=0|\alpha)p(\alpha) = (1-\alpha)p(\alpha)$$

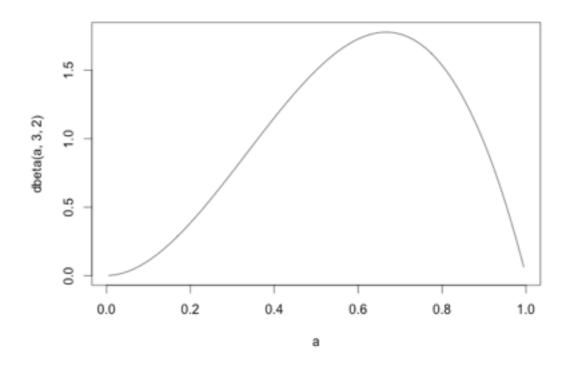


Tossing a coin two times

$$p(\alpha) = 1$$

1.c=0
$$p(\alpha|c=0) = (1-\alpha)$$





Tossing coin - multiple times

$$c = y_i, i = 1..N$$

$$p(\alpha|D) \sim \alpha^{\sum y_i} (1-\alpha)^{N-\sum y_i} p(\alpha)$$

$$p(\alpha) \equiv 1$$

$$p(\alpha|D) \sim \alpha^{\sum y_i} (1-\alpha)^{N-\sum y_i}$$

Beta distribution

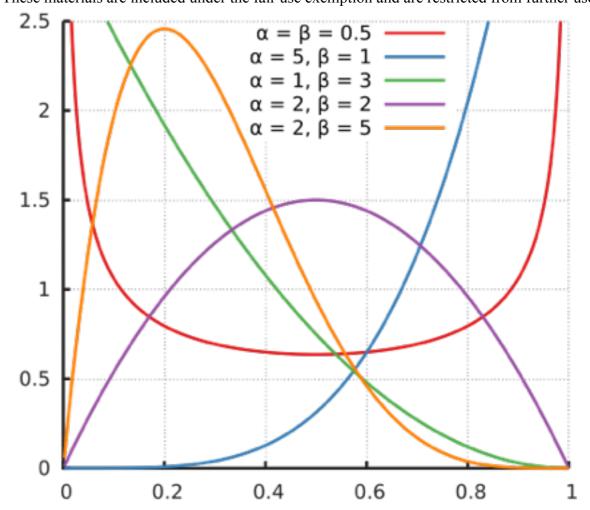
$$Bpdf(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}x^{a-1}(1-x)^{b-1}$$

wikipedia.org

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$$\mu = \frac{a}{a+b}$$

$$\sigma^2 = \frac{ab}{(a+b)^2(a+b+1)}$$





Tossing coin - multiple times

$$p(\alpha) \equiv 1$$
 $p(\alpha|D) \sim \alpha^{\sum y_i} (1 - \alpha)^{N - \sum y_i}$

$$\alpha \sim B\left(1 + \sum y_i, N + 1 - \sum y_i\right)$$

$$p(\alpha) = B(h+1, t+1) - prior$$

$$p(\alpha|y) = B(h + h_2 + 1, t + t_2 + 1)$$

Beta-distribution is conjugate to Bernoulli experiments

Univariate linear regression

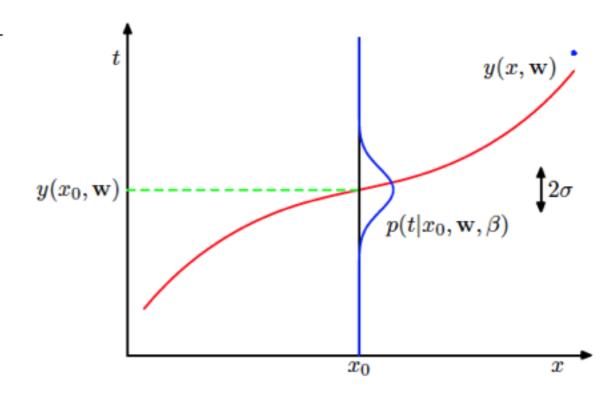
$$y = wx + \varepsilon$$
 $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

$$y \sim \mathcal{N}(wx, \sigma^2)$$
 $D = (Y, X) = \{(y_i, x_i), i = 1..N\}$

ordinary least square (OLS) estimate

$$\sigma = \sqrt{\frac{\sum_{i} (y_i - \hat{w}x_i)^2}{N}}.$$

 $\hat{w} = \frac{\sum_{i} y_i x_i}{\sum_{i} x_i^2}$



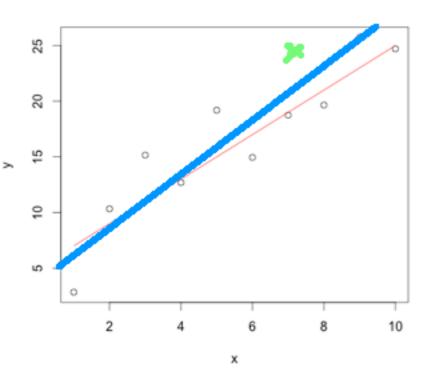
What if we know smth about w?

Bishop, Christopher M. *Pattern recognition and machine learning*. springer, 2006. These materials are included under the fair use exemption and are restricted from further use

Bayesian approach

$$y \sim \mathcal{N}(wx,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(y-wx)^2}{2\sigma^2}} \quad \textbf{\textit{D}} = (\textbf{\textit{Y}},\textbf{\textit{X}}) = \{(\textbf{\textit{y}}_i,\textbf{\textit{x}}_i), \textbf{\textit{i}} = 1..N\}$$
 prior knowledge about $w = w \sim \mathcal{N}(w^*,(\sigma^*)^2) = \frac{1}{\sqrt{2\pi}\sigma^*}e^{-\frac{(w-w^*)^2}{2(\sigma^*)^2}}$

$$p(w|y = y_i, x = x_i) \sim p(y = y_i|w, x = x_i)p(w) \sim e^{-\frac{(y_i - wx_i)^2}{2\sigma^2} - \frac{(w - w^*)^2}{2(\sigma^*)^2}} \sim$$



$$\sim e^{-w^2 \frac{x_i^2(\sigma^*)^2 + \sigma^2}{2\sigma^2(\sigma^*)^2} + w \frac{(\sigma^*)^2 y_i x_i + \sigma^2 w^*}{2\sigma^2(\sigma^*)^2}} \sim e^{-w^2 \frac{x_i^2(\sigma^*)^2 + \sigma^2}{2\sigma^2(\sigma^*)^2} + w \frac{(\sigma^*)^2 y_i x_i + \sigma^2 w^*}{2\sigma^2(\sigma^*)^2}} \sim e^{-w^2 \frac{x_i^2(\sigma^*)^2 + \sigma^2}{2\sigma^2(\sigma^*)^2}}$$

Bayesian approach - adding all observations at once

$$y \sim \mathcal{N}(wx, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-wx)^2}{2\sigma^2}}$$
 $D = (Y, X) = \{(y_i, x_i), i = 1..N\}$

prior knowledge about w

$$w \sim \mathcal{N}(w^*, \sigma^*)$$

$$p(w|Y,X) \sim p(Y|w,X)p(w) = p(w) \prod_{i} p(y = y_i|w, x = x_i) \sim$$

$$\sim e^{-\sum_{i} \frac{(y_{i} - wx_{i})^{2}}{2\sigma^{2}} - \frac{(w - w^{*})^{2}}{2(\sigma^{*})^{2}}} = e^{-\frac{SSE(w)}{2\sigma^{2}} - \frac{(w - w^{*})^{2}}{2(\sigma^{*})^{2}}}$$

$$\hat{w} = \operatorname{argmax}_{w} p(w|Y, X) = \operatorname{argmin}_{w} \left[\frac{RSS(w)}{2\sigma^{2}} + \frac{(w - w^{*})^{2}}{2(\sigma^{*})^{2}} \right]$$

What is the posterior after all?

$$p(w|Y,X) \sim p(Y|w,X)p(w) = p(w) \prod_{i} p(y = y_{i}|w, x = x_{i}) \sim e^{-\sum_{i} \frac{(y_{i} - wx_{i})^{2}}{2\sigma^{2}} - \frac{(w - w^{*})^{2}}{2(\sigma^{*})^{2}}} = e^{-\frac{RSS(w)}{2\sigma^{2}} - \frac{(w - w^{*})^{2}}{2(\sigma^{*})^{2}}}$$

$$p(w|Y,X) \sim e^{-w^2 \frac{\sum_{i} x_i^2(\sigma^*)^2 + \sigma^2}{2\sigma^2(\sigma^*)^2} + w \frac{(\sigma^*)^2 \sum_{i} y_i x_i + \sigma^2 w^*}{2\sigma^2(\sigma^*)^2}} \sim e^{\frac{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2} w^*\right)^2}{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2}\right)^2}} \sim e^{\frac{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2} w^*\right)^2}{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2}\right)^2}} \sim e^{\frac{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2} w^*\right)^2}{\left(\sum_{i} x_i^2 \sigma^{-2} + (\sigma^*)^{-2}\right)^2}}$$

$$\sim \mathcal{N}\left(\frac{\sigma^{-2}\sum_{i}y_{i}x_{i} + (\sigma^{*})^{-2}w^{*}}{\left(\sum_{i}x_{i}^{2}\sigma^{-2} + (\sigma^{*})^{-2}\right)}, \frac{1}{\sqrt{(\sigma^{*})^{-2} + \sum_{i}x_{i}^{2}\sigma^{-2}}}\right)$$

Bayesian approach - uninformed prior

unfinformed prior with $\sigma^* o \infty$

$$p(w|Y,X) \sim e^{-\sum_{i} \frac{(y_i - wx_i)^2}{2\sigma^2} - \frac{(w - w^*)^2}{2(\sigma^*)^2}} = e^{-\frac{RSS(w)}{2\sigma^2} - \frac{(w - w^*)^2}{2(\sigma^*)^2}}$$

$$RSS(w) \rightarrow \min$$

$$w \sim \mathcal{N}\left(\frac{\sigma^{-2} \sum_{i} y_{i} x_{i} + (\sigma^{*})^{-2} w^{*}}{\left(\sum_{i} x_{i}^{2} \sigma^{-2} + (\sigma^{*})^{-2}\right)}, \frac{1}{\sqrt{(\sigma^{*})^{-2} + \sum_{i} x_{i}^{2} \sigma^{-2}}}\right)$$

$$w \sim \mathcal{N}\left(\frac{\sum_{i} x_{i} y_{i}}{\sum_{i} x_{i}^{2}}, \frac{\sigma}{\sqrt{\sum_{i} x_{i}^{2}}}\right)$$

$$\hat{\sigma}^{2} = \frac{RSS(\hat{w})}{N}$$

Multivariate case

$$y \sim \mathcal{N}(w^T x, \sigma^2)$$
 $w = (w_1, w_2, \dots w_n)$

$$D = (Y, X) = \{(y_i, x_i), i = 1..N\}$$

prior knowledge about w

$$w_j \sim \mathcal{N}(w_j^*, \sigma_j^*)$$

$$p(w|Y,X) \sim p(Y|w,X)p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})\prod_{j} p(w_{j}) \sim p(y|w,X)p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})\prod_{j} p(w_{j}) \sim p(y|w,X)p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})\prod_{j} p(w_{j}) \sim p(y|w,X)p(w) = \prod_{i} p(y = y_{i}|w, x = x_{i})p(w) = \prod_{i}$$

$$\sim \prod_{i} e^{\frac{-(y_{i} - w^{T} x_{i})^{2}}{2\sigma^{2}}} \prod_{j} e^{-\frac{(w_{j} - w_{j}^{*})^{2}}{2(\sigma_{i}^{*})^{2}}} = e^{-\frac{RSS(w)}{2\sigma^{2}} - \sum_{j} \frac{(w_{j} - w_{j}^{*})^{2}}{2(\sigma_{i}^{*})^{2}}}$$

$$\hat{w} = argmax_w p(w|Y, X) = argmin_w \left[\frac{RSS(w)}{\sigma^2} + \sum_j \frac{(w_j - w_j^*)^2}{(\sigma_j^*)^2} \right]$$



Overfitting

Area	Month	Price
1010	1	90000
2000	2	200000
2990	3	310000

Price=-1000*Area+1.100.000*Month

Area	Month	Price
1500	12	150000

Price=-1000*1500+ 1.1M*12=11.7M?

Ridge and Lasso regression

Require coefficients to be not too big

$$\hat{w} = argmax_w p(w|Y, X) = argmin_w \left[\frac{RSS(w)}{\sigma^2} + \sum_j \frac{(w_j - w_j^*)^2}{(\sigma_j^*)^2} \right]$$

$$w_j \sim \mathcal{N}(0, \sigma/\sqrt{\lambda})$$

$$\hat{w} = argmin_w \left[RSS(w) + \lambda ||w||_2^2 \right]$$

$$\|w\|_2 = \sqrt{\sum_j w_j^2}$$

Laplacian prior distribution $p(w_i) \sim e^{-\lambda |w_j|/\sigma}$

$$\hat{w} = argmin_w \left[RSS(w) + \lambda ||w||_1 \right]$$

$$\|w\|_1 = \sum_j |w_j|$$

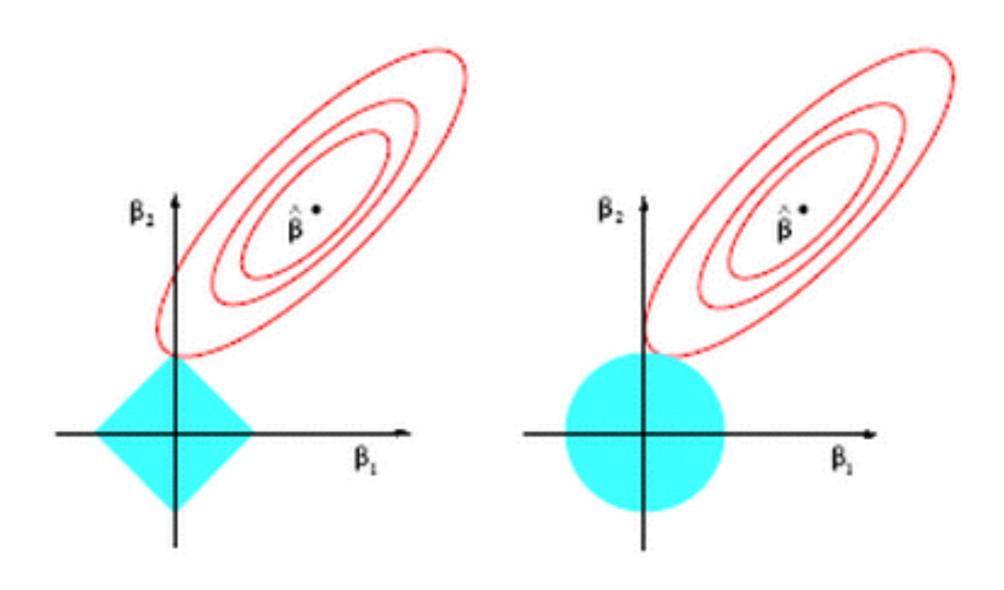
$$RSS(w) \rightarrow min, ||w||_p \leq \alpha$$

Ridge regression admits solution in the closed form

$$\hat{w} = (X^T X + \lambda I)^{-1} X^T Y$$



Ridge and Lasso regression





Fighting overfitting

Area	Month	Price
1010	1	90000
2000	2	200000
2990	3	310000

```
Lasso (lambda=1): Price=88.34*Area+13212.5*Month Lasso (lambda=50): Price=98.77*Area+2787.1*Month Lasso (lambda=100): Price=101.56*Area+0*Month
```

Area	Month	Price
1500	12	150000



Criticism

- Dependence on the subjective prior
- Where do we get the prior?
- Computational complexity
- Universal? No free lunch!