CS189/CS289A
Introduction to Machine Learning
Lecture 9: Regression

Peter Bartlett

February 17, 2015

Outline

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- Review: Decision theory.

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- Empirical risk minimization.

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Review: Quadratic loss

Regression with quadratic loss

Outcomes are in $\mathcal{Y} = \mathbb{R}$.
We consider the quadratic loss function, $\ell(\hat{y}, y) = (\hat{y} - y)^2$.
Risk is expected squared error:

$$R(f) = \mathbb{E}\ell(f(X), Y) = \mathbb{E}\left(f(X) - Y\right)^2.$$

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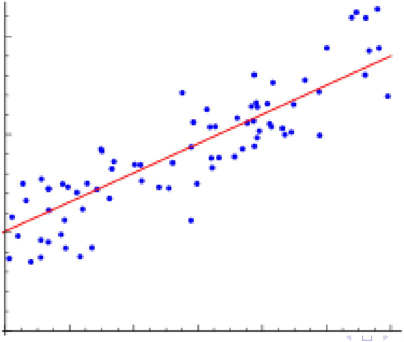

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In both cases, we arrive at the *normal equations*: the choice of β corresponds to a projection on to a linear sub-space.

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Here, $\hat{\mathbb{E}}_n$ means expectation under the *empirical distribution*, which puts mass $1/n$ at each (X_i, Y_i) pair in the sample.

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$$\begin{aligned}\hat{f} &:= \arg\min_{f \in F_{lin}} \hat{\mathbb{E}}_n \ell(f(X), Y) \\ &= \arg\min_{f \in F_{lin}} \sum_{i=1}^{n} (f(X_i) - Y_i)^2.\end{aligned}$$

Linear regression: Least squares

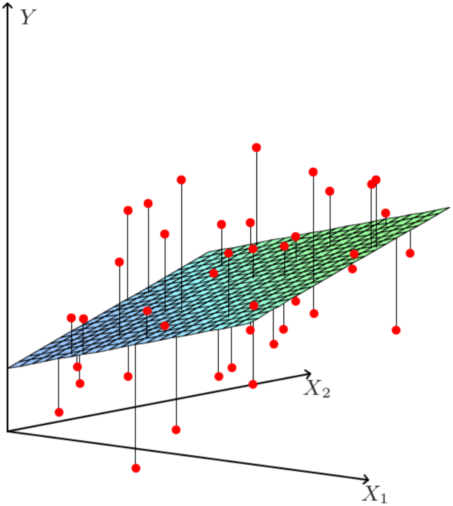

FIGURE 3.1. *Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.*

Linear regression: Least squares

Just as we did when we were considering linear classifiers, we'll simplify notation by bundling the offset term (β_0) into the parameter vector β and assuming that the covariates X_i include a constant 1 component.

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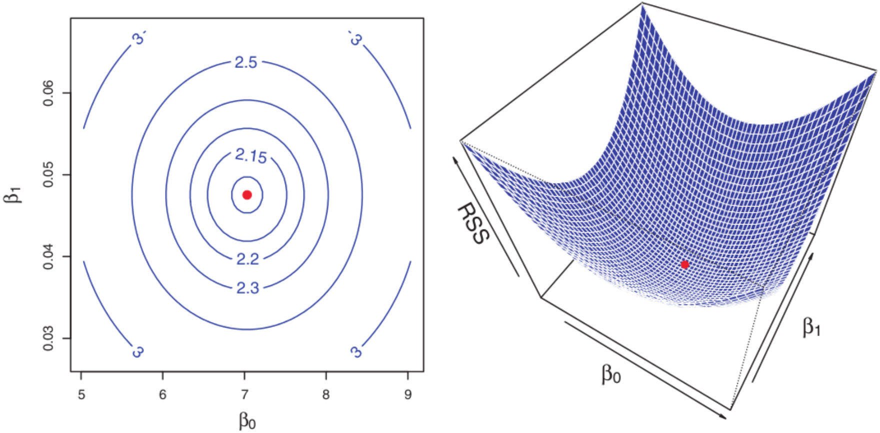
$$\begin{aligned}\hat{\beta} &= \arg\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^{n} (X_i'\beta - Y_i)^2 \\ &= \arg\min_{\beta \in \mathbb{R}^p} \underbrace{\|X\beta - y\|^2}_{\text{RSS}},\end{aligned}$$

where the *design matrix* $X \in \mathbb{R}^{n \times p}$ and response vector $y \in \mathbb{R}^n$ are

$$X = \begin{pmatrix} X_1' \\ X_2' \\ \vdots \\ X_n' \end{pmatrix}, \qquad y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}.$$

(Think of $n \gg p$, so X is tall.)

Linear regression: Least squares



Linear regression: Least squares

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Linear regression: Least squares

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we have

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That is, we want to find a linear combination of the columns $x_j \in \mathbb{R}^n$ of X that minimizes Euclidean distance to $y \in \mathbb{R}^n$.

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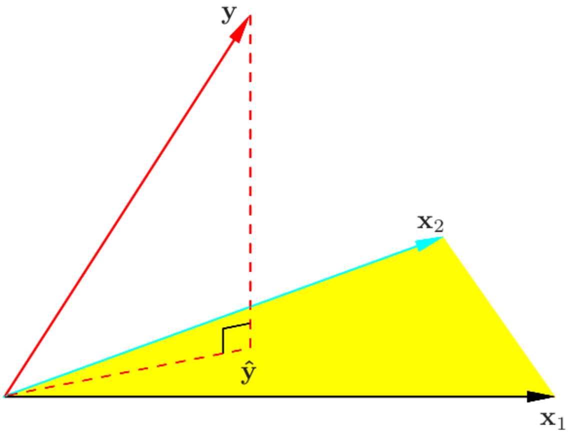

FIGURE 3.2. *The N-dimensional geometry of least squares regression with two predictors. The outcome vector $\mathbf{y}$ is orthogonally projected onto the hyperplane spanned by the input vectors $\mathbf{x}_1$ and $\mathbf{x}_2$. The projection $\hat{\mathbf{y}}$ represents the vector of the least squares predictions*

Linear regression: Least squares

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4. $n \gg p$.

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Linear regression: probability models

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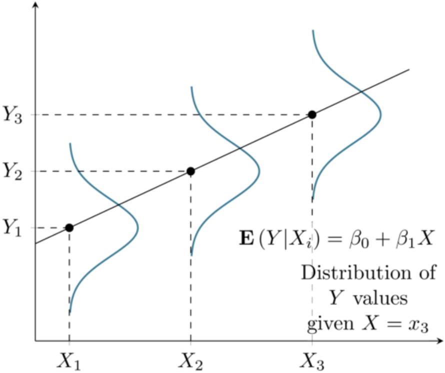

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(see text)

Outline

- Review: Decision theory.
- Empirical risk minimization.
  - Least squares.
  - Normal equations.
- Linear model with additive Gaussian noise.
  - Maximum likelihood is least squares.
  - Distributions of parameter estimates.