Linear regression through Optimization

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Outline

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Generalizing Linear regression to multiple variables

Measuring the fitness of linear models

Extending the linear regression procedure

If you have data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_P, y_P)$ where, for some $N > 1$ the input $\mathbf{x}_i$ is a vector in $\mathbb{R}^N$, can you still do linear regression?

Extending the linear regression procedure

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For each i with $1 \leq i \leq P$, say that $\mathbf{x}_i = \begin{bmatrix} x_{1,i} \\ x_{2,i} \\ \vdots \\ x_{N,i} \end{bmatrix}$. Define a $P \times \left(N + 1\right)$ matrix A so that the i^{th} row is $\left[1, x_{1,i}, x_{2,i}, \ldots, x_{N,i}\right]$.

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In other words, set $\tilde{\mathbf{x}}_i$ equal to the vector in $\mathbb{R}^{N+1}$ with 1 as its first component and $\mathbf{x}_i$ for the remaining N components. Then

$$A = \begin{bmatrix} — & \tilde{\mathbf{x}}_1^T & — \\ — & \tilde{\mathbf{x}}_2^T & — \\ & \vdots & \\ — & \tilde{\mathbf{x}}_P^T & — \end{bmatrix}.$$

Extending the linear regression procedure

A solution $\tilde{\mathbf{w}}^\star = [b^\star, w_1^\star, \ldots, w_N^\star]^T$ to the normal equations $A^T A \tilde{\mathbf{w}} = A^T \mathbf{y}$ (with A as above) gives coefficients for a linear model for the data.[1]

[1] The matrix $A^T A$ is $(N+1) \times (N+1)$ and $A^T \mathbf{y}$ is a vector in $\mathbb{R}^{N+1}$.

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Write $\mathbf{w}^\star \in \mathbb{R}^N$ for the non-constant coefficient vector $\left[w_1^\star, w_2^\star, \ldots, w_N^\star\right]^T$. The affine linear model on the data, in N variables, is

$$f_{\tilde{\mathbf{w}}^\star}(\mathbf{x}) = b^\star + w_1^\star x_1 + \ldots + w_N^\star x_N = b^\star + \mathbf{x}^T\mathbf{w}^\star.$$

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(1) $f_{\tilde{\mathbf{w}}^\star}(\mathbf{x})$ is affine linear, meaning the difference in two function values is a dot product on the difference of the input. Specifically, $f_{\tilde{\mathbf{w}}^\star}(\mathbf{x}) - f_{\tilde{\mathbf{w}}^\star}(\mathbf{x}') = (\mathbf{x} - \mathbf{x}')^T\mathbf{w}^\star$.

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(2) The graph of $f_{\tilde{\mathbf{w}}^\star}(\mathbf{x})$ is a hyperplane[2] in $\mathbb{R}^{N+1}$ with normal vector $\left[1, -w_1^\star, \ldots, -w_N^\star\right]^T$.

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Example

A concrete example: using the data in `'Advertising.csv'`, found in the DataSets folder of the course site.

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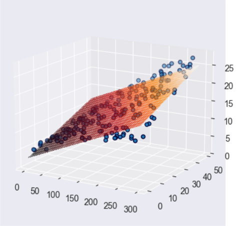
To perform linear regression, with independent variables `'TV'`, `'Radio'`, and `'Newspaper'` and setting y equal to `'Sales'`, one may follow the procedure above. The matrix A described is 200×4 ($N = 3$). The resulting coefficients are (approximately)



3D projection of Advertising model

$$[b^\star, w_1^\star, w_2^\star, w_3^\star] = [2.9389, 0.0458, 0.1885, -0.001].$$

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“Noise” and linear regression model

Underlying assumption: the (input) variables $x_1, \ldots, x_N$ are not random, but there is natural variability in the “y-direction” (value of $f_{\tilde{\mathbf{w}}}$), represented with a random variable.[3]

[3]Note that, if you instead consider the random variable to be in another direction (swapping some x_j with y) then there is a *different* linear regression.

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So, there is a b and $\mathbf{w} = [w_1, \ldots, w_N]^T$, so that the relationship between $\mathbf{x}$ and y is

$$y = b + \mathbf{x}^T\mathbf{w} + \varepsilon,$$

where ε is a random variable with mean (first moment) equal to 0.

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- A common consideration: ε normally distributed.

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Least Squares loss function

On given data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_P, y_P)$, a common measure for how well a linear regression model fits is the **Mean Squared Error**. If the intercept and $\mathbf{w}$ vector for the regression line are $b^\star$ and $\mathbf{w}^\star$ then we have $\hat{y}_i = b^\star + \mathbf{x}_i^T \mathbf{w}^\star$ and the Mean Squared Error is

$$\frac{1}{P}\sum_{i=1}^{P}\left(\hat{y}_i - y_i\right)^2 = \frac{1}{P}\sum_{i=1}^{P}\left(b^\star + \mathbf{x}_i^T \mathbf{w}^\star - y_i\right)^2.$$

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It is helpful to think of this as a function on an arbitrary choice of parameters $\tilde{\mathbf{w}} = (b, \mathbf{w})$. Dropping the division by P, this is the **Least Squares loss** function: if $f_{\tilde{\mathbf{w}}}(\mathbf{x}) = b + \mathbf{x}^T \mathbf{w}$ is the linear model for parameters $\tilde{\mathbf{w}} = (b, w_1, \ldots, w_N)$ then this loss function is

$$g(\tilde{\mathbf{w}}) = \sum_{i=1}^{P} \left(f_{\tilde{\mathbf{w}}}(\mathbf{x}_i) - y_i\right)^2 .$$

Minimizing the Least Squares loss

For fixed data $\left\{\left(\mathbf{x}_i, y_i\right)\right\}_{i=1}^{P}$, how do we solve the problem

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We can use methods from calculus to determine the minimum (and the minimizer, to set equal to $\tilde{\mathbf{w}}$). Specifically, the first order condition is useful – that we want a value of $\tilde{\mathbf{w}}$ where all partial derivatives of $g\left(\tilde{\mathbf{w}}\right)$ are equal to zero.

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Next: a review of calculus minimization techniques.

Meaning of Least Squares loss

For $1 \le i \le P$, the quantity $\left|f_{b,\mathbf{w}}(\mathbf{x}_i) - y_i\right|$ is the vertical distance from $(\mathbf{x}_i, y_i)$ to the point predicted by the linear model, $(\mathbf{x}_i, f_{\tilde{\mathbf{w}}}(\mathbf{x}_i))$.

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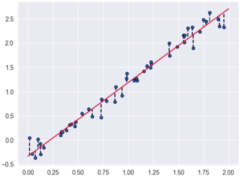

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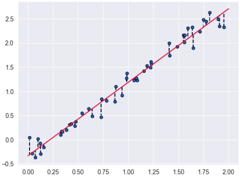

The length of the vector $\mathbf{y} - \hat{\mathbf{y}}$ (*i.e.*, the distance from $\mathbf{y}$ to the vector of predictions, in the column space of our feature matrix) is equal to

$$\sqrt{(f_{\tilde{\mathbf{w}}}(\mathbf{x}_1) - y_1)^2 + (f_{\tilde{\mathbf{w}}}(\mathbf{x}_2) - y_2)^2 + \ldots + (f_{\tilde{\mathbf{w}}}(\mathbf{x}_P) - y_P)^2} = \sqrt{g(\tilde{\mathbf{w}})}.$$

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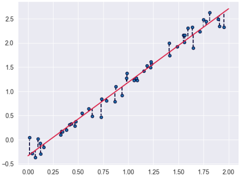

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We see that minimizing $g(\tilde{\mathbf{w}})$ is the same as minimizing that distance, giving the $\hat{\mathbf{y}}$ in the column space that makes $\mathbf{y} - \hat{\mathbf{y}}$ orthogonal to the column space.