EECS 545: Machine Learning
Lecture 3. Linear Regression (part 2)

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Regularized Linear Regression

Back to Polynomial Coefficients

	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Underfitting

Good

Overfitting;
Coefficients are large!

$$h(x,\mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{M-1} x^{M-1}$$

Regularized Least Squares (1)

- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization

λ is called the regularization coefficient.

- With the sum-of-squares error function and a quadratic regularizer, we get

Penalize large coefficient values

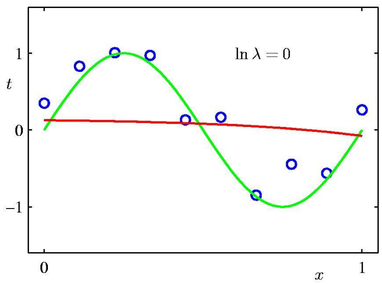
$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

New objective function

Definition (L2): $\|\mathbf{w}\|_2^2 = \sum_{j=0}^{M-1} w_j^2$

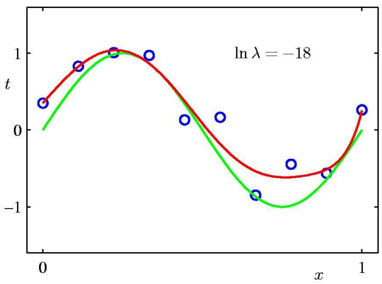
- Effect of λ

L2 Regularization: $\ln\lambda = 0$



$M = 9$ $\quad \widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$

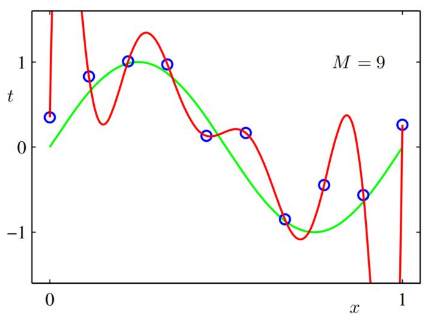
L2 Regularization: $\ln\lambda = -18$



$M = 9$ $\quad \widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$

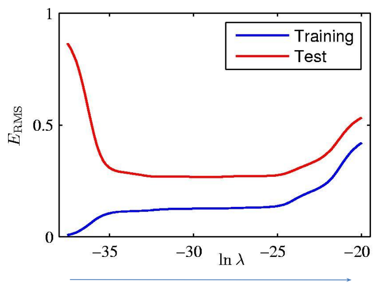
"No" L2 Regularization: $\lambda = 0$

(or when L2 regularization is too small) $\quad$ (or $\ln\lambda \to -\infty$)



$M = 9$ $\quad \widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \cancel{\frac{\lambda}{2}\|\mathbf{w}\|_2^2}$

L2 Regularization: E_{RMS} vs. $\ln\lambda$



Larger regularization

$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

NOTE: For simplicity of presentation, we divided the data into training set and test set. However, it's **not** legitimate to find the optimal hyperparameter based on the test set. We will talk about legitimate ways of doing this when we cover model selection and cross-validation.

Polynomial Coefficients

(i.e., λ = 0)

	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Overfitting; Coefficients are large! | Good | Underfitting

Regularized Least Squares (1)

- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization

λ is called the regularization coefficient.

- With the sum-of-squares error function and a quadratic regularizer, we get

Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

- Closed-form solution:

$$\mathbf{w}_{\text{reg}} = (\lambda\mathbf{I} + \Phi^\top\Phi)^{-1}\Phi^\top\mathbf{y}$$

Derivation

Objective function

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

$$= \frac{1}{2}\mathbf{w}^\top\Phi^\top\Phi\mathbf{w} - \mathbf{w}^\top\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

Compute the gradient and set it zero:

$$\nabla_{\mathbf{w}}\widetilde{E}(\mathbf{w}) = \nabla_{\mathbf{w}}\left[\frac{1}{2}\mathbf{w}^\top\Phi^\top\Phi\mathbf{w} - \mathbf{w}^\top\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}\right]$$

$$= \Phi^\top\Phi\mathbf{w} - \Phi^\top\mathbf{y} + \lambda\mathbf{w}$$

$$= (\lambda\mathbf{I} + \Phi^\top\Phi)\mathbf{w} - \Phi^\top\mathbf{y}$$

$$= 0$$

$$\mathbf{w}_{\text{ML}} = (\Phi^\top\Phi)^{-1}\Phi^\top\mathbf{y}$$

v.s. Ordinary Least Square

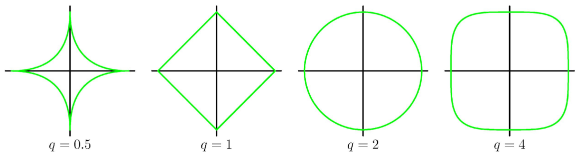
Therefore, we get: $\mathbf{w}_{\text{reg}} = (\lambda\mathbf{I} + \Phi^\top\Phi)^{-1}\Phi^\top\mathbf{y}$

Regularized Least Squares (2)

- With a more general regularizer, we have

$$\frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

Note: In this lecture, we focus on q=2 (L2 regularization), but other values of q>0 can be used.

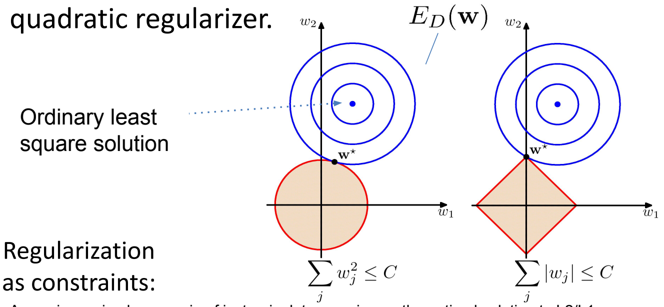


Lasso "L1 regularization" | Quadratic "L2 regularization"

plotting curves of (w_1, w_2) where $\sum_{j=1}^{M}|w_j|^q$ is a constant. (M=2)

Regularized Least Squares (3)

- Lasso tends to generate sparser solutions than a quadratic regularizer.



Assuming a simple scenario of isotropic data covariance, the optimal solution to L2/L1 regularization is closest point to the original solution (center of the concentric circles) that touches the boundary of the L2/L1 constraint.

Summary: Regularized Linear Regression

- Simple modification of linear regression
- Regularization controls the tradeoff between "fitting error" and "complexity"
  - Small regularization results in complex models (but with risk of overfitting)
  - Large regularization results in simple models (but with risk of underfitting)
- It is important to find an optimal regularization that balances between the two.

Maximum Likelihood interpretation of least squares regression

Review on probability

Probability: Terminology

- **Experiment**: Procedure that yields an outcome
  - E.g., Tossing a coin three times:
    - Outcome: HHH in one trial, HTH in another trial, etc.
- **Sample space**: Set of all possible outcomes in the experiment, denoted as Ω (or S)
  - E.g., for the above example:
    - Ω = {HHH, HHT, HTH, HTT, THH, THT, THT, TTH, TTT}
- **Event**: subset of the sample space Ω (i.e., an event is a set consisting of individual outcomes)
  - Event space: Collection of all events , called $\mathcal{F}$ (aka σ-algebra)
  - E.g., Event that # of heads is an even number.
    - E = {HHT, HTH, THH, TTT}
- **Probability measure**: function (mapping) from events to probability levels. I.e., $P : \mathcal{F} \rightarrow [0, 1]$ (see next slide)
  - Probability that # of heads is an even number: 4/8 = 1/2.
- **Probability space**: (Ω, $\mathcal{F}$, P)

Law of Total Probability

$$P(A) \geq 0, \forall A \in \mathcal{F}$$
$$P(\Omega) = 1$$

- Law of total probability

$$P(A) = P(A \cap B) + P(A \cap B^C)$$

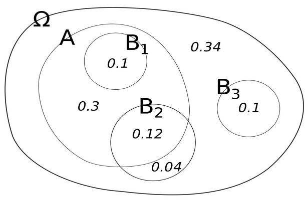
$$P(A) = \sum_i P(A \cap B_i) \quad \text{Discrete } B_i$$

$$P(A) = \int P(A \cap B_i) dB_i \quad \text{Continuous } B_i$$

Conditional Probability

For events $A, B \in \mathcal{F}$ with $P(B) > 0$, we may write the **conditional probability** of A given B:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$



From Wikipedia

$$P(A|B_1) = 1$$
$$P(A|B_2) = 0.12/(0.12 + 0.04) = 0.75$$
$$P(A|B_3) = 0 \quad \text{(disjoint)}$$
$$P(A) = 0.30 + 0.10 + 0.12 = 0.52$$
(the unconditional probability)

Bayes' Rule

Using the chain rule we may see:

$$P(A|B)P(B) = P(A \cap B) = P(B|A)P(A)$$

Rearranging this yields **Bayes' rule:**

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

Often this is written as:

$$P(B_i|A) = \frac{P(A|B_i)P(B_i)}{\sum_i P(A|B_i)P(B_i)}$$

Where B_i are a partition of Ω (note the bottom is just the law of total probability).

Likelihood Functions

Why is Bayes' so useful in learning? Allows us to compute the posterior of **w** given data D:

$$p(\mathbf{w}|D) = \frac{p(D|\mathbf{w})p(\mathbf{w})}{p(D)}$$

Prior

Posterior

Bayes' rule in words: posterior ∝ likelihood × prior

$$p(\mathbf{w}|D) \propto p(D|\mathbf{w})p(\mathbf{w})$$

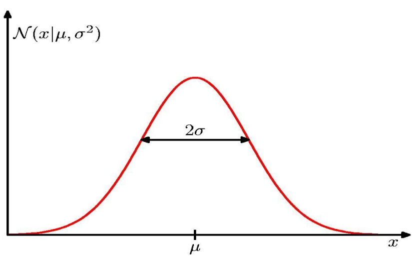
The likelihood function, $p(\mathbf{w} \mid D)$, is evaluated for observed data D as a function of **w**. It expresses how parameter settings **w**.

Maximum Likelihood Estimation (MLE)

- Maximum likelihood:
  - choose parameter setting **w** that maximizes likelihood function $p(D \mid \mathbf{w})$.
  - choose the value of **w** that maximizes the probability of observed data.
- Cf. MAP (Maximum a posteriori) estimation
  - Equivalent to maximizing $p(\mathbf{w}|D) \propto p(D|\mathbf{w})p(\mathbf{w})$
  - Can compute this using Bayes rule!
  - This will be covered in later lectures

The Gaussian Distribution

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



$$\mathcal{N}(x|\mu, \sigma^2) > 0$$

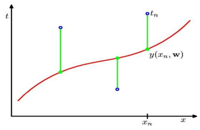
$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2)\, \mathrm{d}x = 1$$

Maximum Likelihood interpretation of least squares regression

MLE for Linear Regression

- Assume a stochastic model:

$$y^{(n)} = \mathbf{w}^\top \phi(\mathbf{x}^{(n)}) + \epsilon \qquad \text{where } \epsilon \sim \mathcal{N}(0, \beta^{-1})$$



- This gives a likelihood function:

$$p(y^{(n)} \mid \phi(\mathbf{x}^{(n)}), \mathbf{w}, \beta) = \mathcal{N}(y^{(n)} \mid \mathbf{w}^\top \phi(\mathbf{x}^{(n)}), \beta^{-1})$$

- With input matrix $\mathbf{\Phi}$ and output matrix $\mathbf{y}$, the data likelihood is:

$$p(\mathbf{y} \mid \mathbf{\Phi}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(y^{(n)} \mid \mathbf{w}^\top \phi(\mathbf{x}^{(n)}), \beta^{-1})$$

Log-likelihood

- Given data likelihood (prev. slide)

$$p(\mathbf{y} \mid \mathbf{\Phi}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(y^{(n)} \mid \mathbf{w}^\top \phi(\mathbf{x}^{(n)}), \beta^{-1})$$

- Log likelihood:

$$\log p(\mathbf{y}|\mathbf{\Phi}, \mathbf{w}, \beta) = \frac{N}{2}\log\beta - \frac{N}{2}\log 2\pi - \beta E_D(\mathbf{w})$$

where $E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$

- Derivation?

Derivation of log-likelihood of p

From $p(y^{(n)} \mid \phi(\mathbf{x}^{(n)}), \mathbf{w}, \beta) = \mathcal{N}(y^{(n)} \mid \mathbf{w}^\top \phi(\mathbf{x}^{(n)}), \beta^{-1})$

$$= \sqrt{\frac{\beta}{2\pi}}\exp\left(-\frac{\beta}{2}\left\|y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})\right\|^2\right)$$

Derive: $\log p(y^{(1)}, y^{(2)}, \ldots, y^{(N)} \mid \mathbf{\Phi}, \mathbf{w}, \beta)$

$$= \log \prod_{n=1}^{N} \mathcal{N}\left(y^{(n)} \mid \mathbf{w}^\top\phi(\mathbf{x}^{(n)}), \beta^{-1}\right)$$

$$= \sum_{n=1}^{N} \log\left(\sqrt{\frac{\beta}{2\pi}}\exp\left(-\frac{\beta}{2}\left\|y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})\right\|^2\right)\right)$$

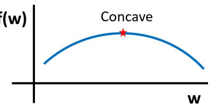
$$= \sum_{n=1}^{N}\left(\frac{1}{2}\log\beta - \frac{1}{2}\log 2\pi - \frac{\beta}{2}\left\|y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})\right\|^2\right)$$

$$= \frac{N}{2}\log\beta - \frac{N}{2}\log 2\pi - \sum_{n=1}^{N}\frac{\beta}{2}\left\|y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})\right\|^2$$

Maximum likelihood estimation (MLE)

- Let's maximize the log-likelihood!
- Set the gradient of log-likelihood = 0 (Why?)

$$\nabla_{\mathbf{w}} \log p(y|\mathbf{\Phi}, \mathbf{w}, \beta) = \nabla_{\mathbf{w}}\left(\underbrace{\frac{N}{2}\log\beta - \frac{N}{2}\log 2\pi}_{\text{Constant}} - \sum_{n=1}^{N}\frac{\beta}{2}\left\|y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})\right\|^2\right)$$



$$= \beta\sum_{n=1}^{N}\left(\underbrace{y^{(n)} - \mathbf{w}^\top\phi(\mathbf{x}^{(n)})}_{\text{Scalar}}\phi(\mathbf{x}^{(n)})\right)$$

$$= \beta\left(\sum_{n=1}^{N} y^{(n)}\phi(\mathbf{x}^{(n)}) - \phi(\mathbf{x}^{(n)})\phi(\mathbf{x}^{(n)})^\top\mathbf{w}\right) = 0$$

- In matrix form, $\beta(\Phi^\top\mathbf{y} - \Phi^\top\Phi\mathbf{w}) = 0$

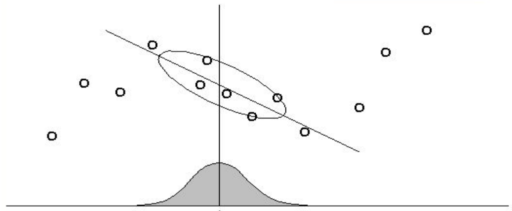
$$\mathbf{w}_{\text{ML}} = (\Phi^\top\Phi)^{-1}\Phi^\top\mathbf{y}$$

- MLE solution is equivalent to OLS solution!

Locally-weighted Linear Regression

Locally weighted linear regression

- Main idea: When predicting $f(\hat{\mathbf{x}})$, give high weights for "neighbors" of $\hat{\mathbf{x}}$.

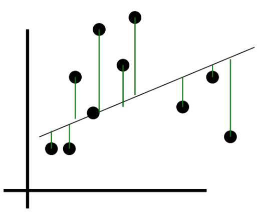


$\hat{\mathbf{x}}$

In locally weighted regression, points are weighted by proximity to the current $\hat{\mathbf{x}}$ in question using a kernel. A regression is then computed using the weighted points.

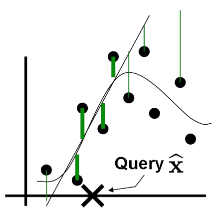
Slide credit: William Cohen

Regular linear regression vs. locally weighted linear regression



Regular linear regression

$$\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$$



Locally weighted linear regression

$$\sum_{n=1}^{N} r^{(n)}(\hat{\mathbf{x}})\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$$

Linear regression vs. Locally-weighted Linear Regression

- A query point $\hat{\mathbf{x}}$, training set $\left\{\left(\mathbf{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$
- Linear regression
  1. Fit $\mathbf{w}$ to minimize $\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$
  2. Predict $\mathbf{w}^\top\phi(\hat{\mathbf{x}})$
- Locally-weighted linear regression
  1. Fit $\mathbf{w}$ to minimize $\sum_{n=1}^{N} r^{(n)}(\hat{\mathbf{x}})\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$
  2. Predict $\mathbf{w}^\top\phi(\hat{\mathbf{x}})$

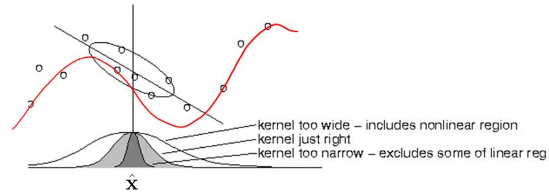
weights are dependent on the query $\hat{\mathbf{x}}$
(i.e., need to solve the optimization for each query value)

Linear regression vs. Locally-weighted Linear Regression

- Locally-weighted linear regression
  1. Fit $\mathbf{w}$ to minimize $\sum_{n=1}^{N} r^{(n)}(\widehat{\mathbf{x}}) \left(\mathbf{w}^\top \phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2$
  2. Predict $\mathbf{w}^\top \phi(\widehat{\mathbf{x}})$
- Remarks:
  1. Standard choice: $r^{(n)}(\widehat{\mathbf{x}}) = \exp\left(-\frac{\left\|\phi(\mathbf{x}^{(n)}) - \phi(\widehat{\mathbf{x}})\right\|^2}{2\tau^2}\right)$ Gaussian kernel with kernel width τ
  2. Note that $r^{(n)}(\widehat{\mathbf{x}})$ depends on $\widehat{\mathbf{x}}$ (query point), and you solve linear regression for each query point $\widehat{\mathbf{x}}$
  3. The problem can be formulated as a modified version of least squares problem (HW#1)

Locally weighted linear regression

- Choice of kernel width τ matters
  - Requires hyper-parameter tuning



The estimator is minimized when kernel includes as many training points as can be accommodated by the model. Too large a kernel includes points that degrade the fit; too small a kernel neglects points that increase confidence in the fit.

Slide credit: William Cohen

Summary

- L_2 Regularized linear regression $\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{w}^\top\phi(\mathbf{x}^{(n)}) - y^{(n)}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$
  - Adding L_2 regularizer
  - Can be solved via closed form (simple modification of the original linear regression)
  - penalizes complex solutions (with high weights)
- Maximum likelihood interpretation of linear regression
  - Linear regression can be interpreted as performing MLE assuming the Gaussian noise distribution for targets
- Locally-weighted linear regression