Computer Science

CSC480/580: Principles of Machine Learning

Linear Models

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Recap of last 2 lectures

- Classification performance beyond error rates
  - How is TPR defined?
  - How is ROC curve defined?
- Reliable model evaluation & comparison
  - Confidence interval
  - Hypothesis testing
- Debugging ML algorithms
  - Assessing data size & quality
  - Learning algorithm implementation
- Bias-variance tradeoff

Outline

- Linear Models for Regression
  - Least Squares Estimation
  - Regularized Least Squares
- Linear Models for Classification
  - Logistic Regression
  - Support Vector Machine

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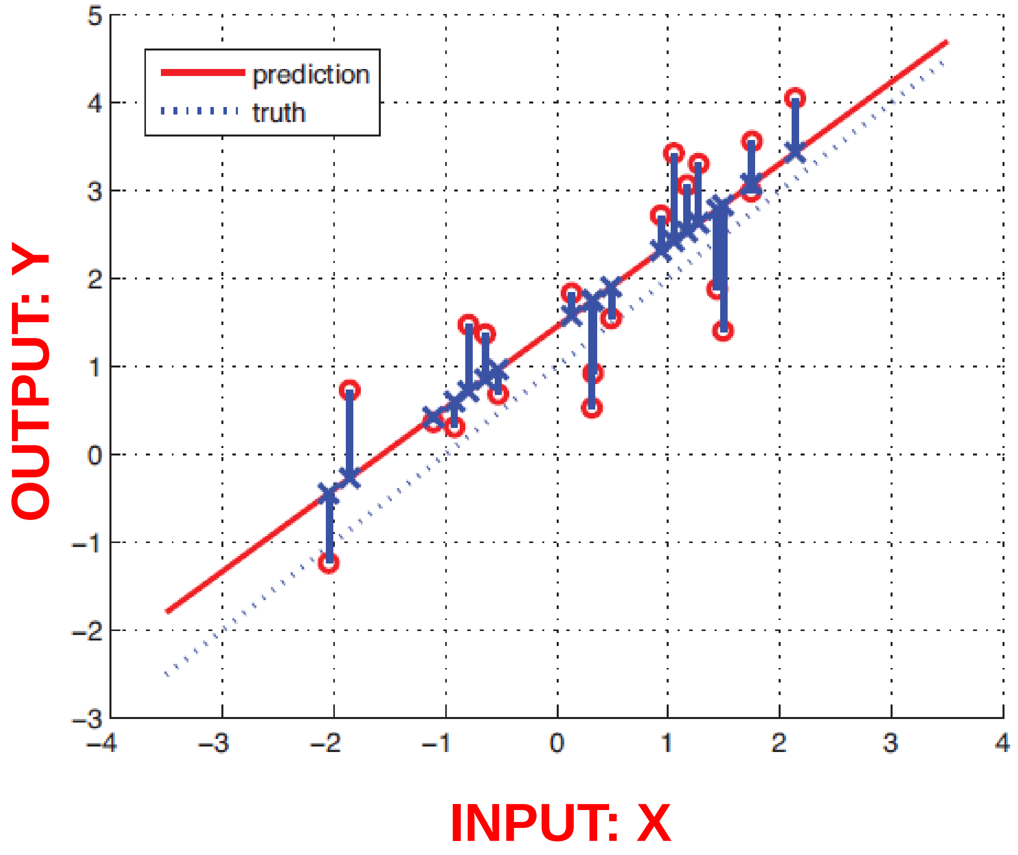
Linear Regression



Regression Learn a function that predicts outputs from inputs,

$$y = f(x)$$

Outputs y are real-valued

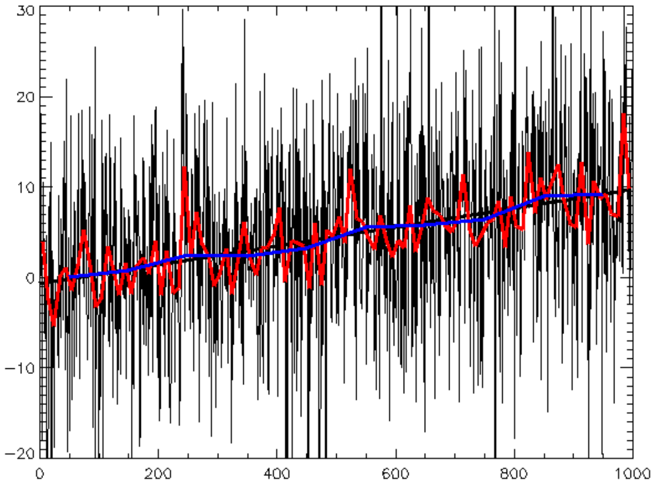
Linear Regression As the name suggests, uses a *linear function*:

$$y = w^T x + b$$

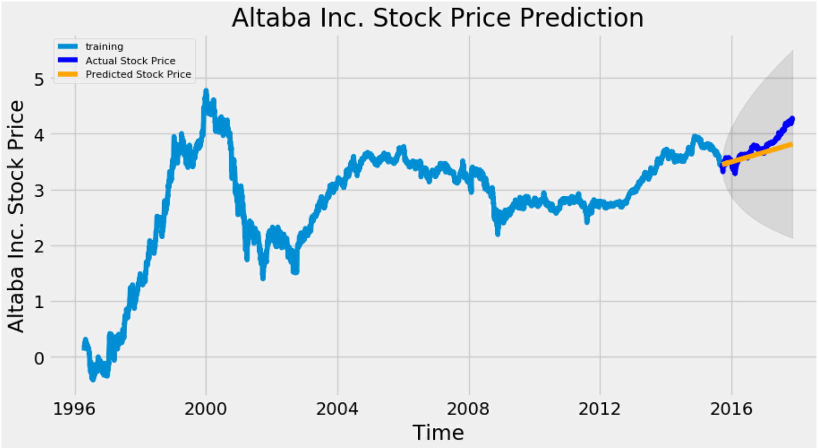
We will consider noise in data later…

Linear Regression

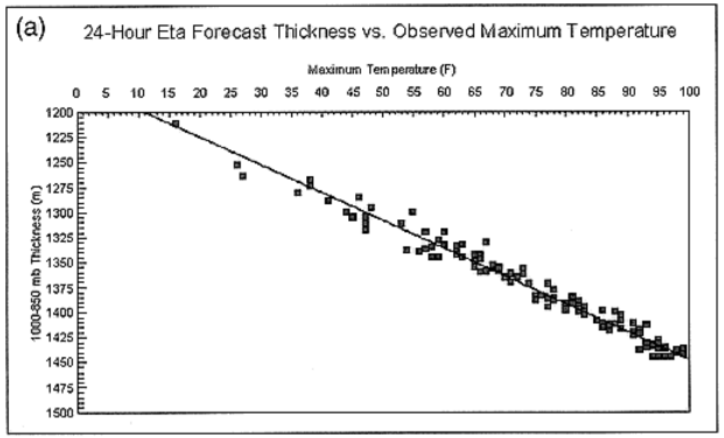
Where is linear regression useful?



Trendlines



Stock Prediction

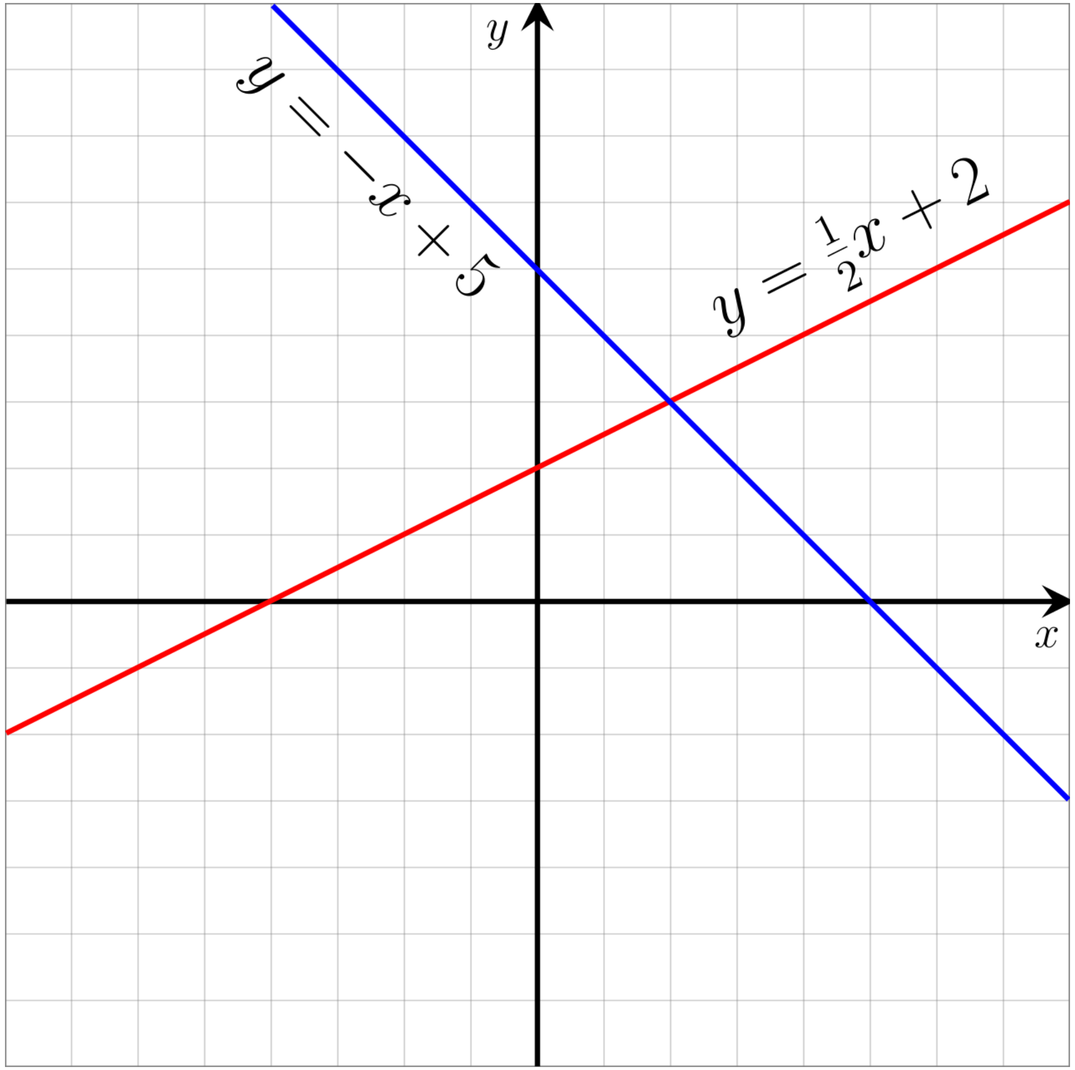


Climate Models

Massie and Rose (1997)

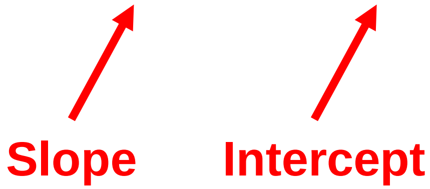
Used anywhere a linear relationship is assumed between continuous inputs / outputs

Line Equation



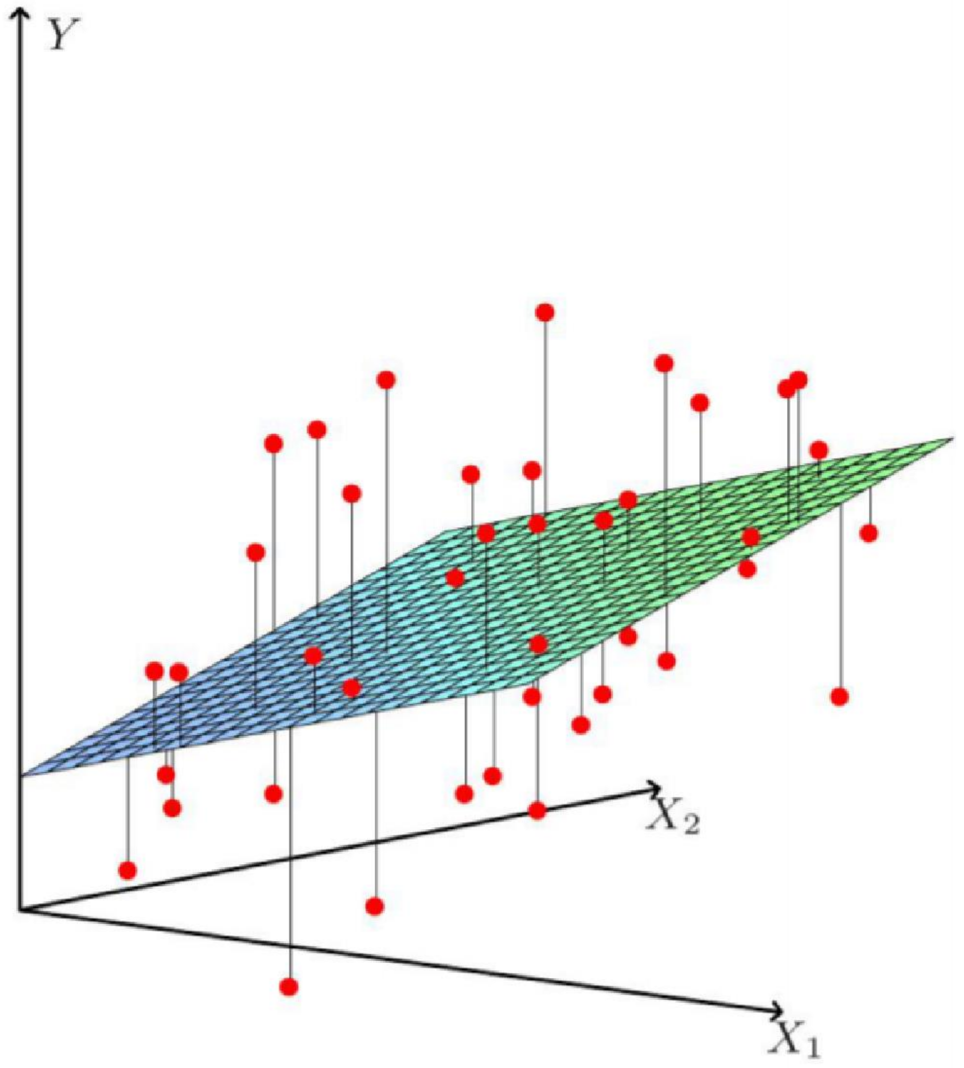
Recall the equation for a line has a *slope* and an *intercept*,

$$y = w \cdot x + b$$



- Intercept (b) indicates where line crosses y-axis
- Slope controls angle of line
- Positive slope (w) → Line goes up left-to-right
- Negative slope → Line goes down left-to-right

Linear regression in dimension >= 2



$$h(x) = w_1 \cdot x_1 + w_2 \cdot x_2 + b = \langle w, x \rangle + b$$

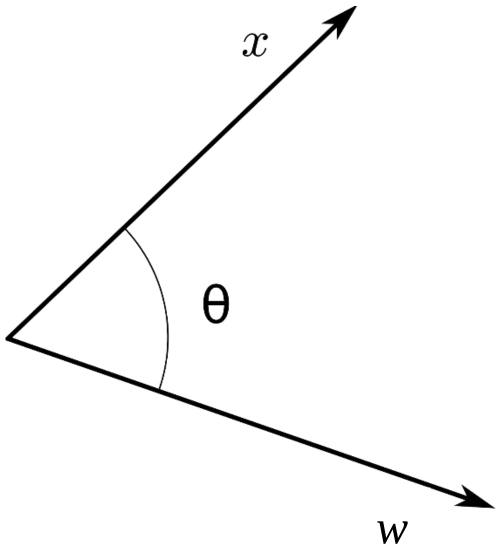
$y = \langle w, x \rangle + b$ can be viewed as a hyperplane

Inner Products

Recall the definition of an *inner product*:

$$w^T x = w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$$

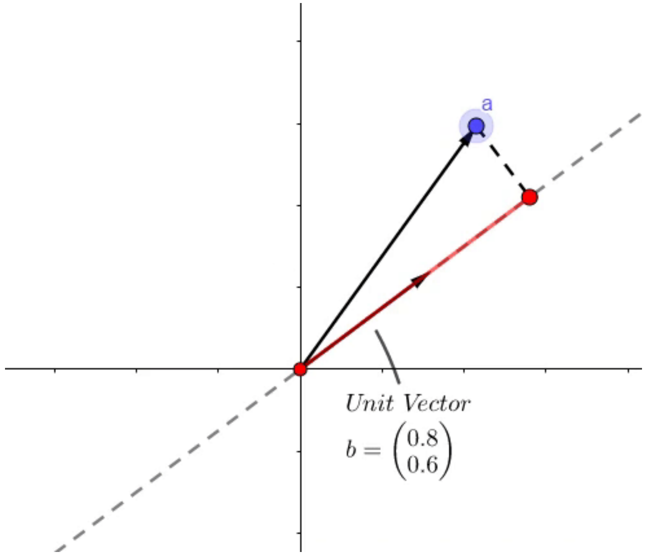
$$= \sum_{d=1}^{D} w_d x_d$$



Projection of one vector onto another,

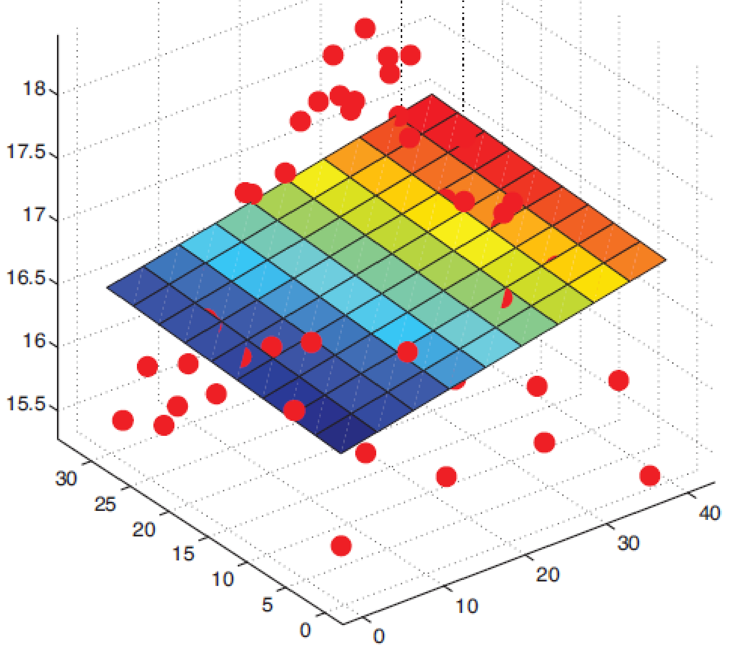
$$w^T \hat{x} = |w| \cos\theta$$ where $$\hat{x} = \frac{x}{|x|} = \frac{x}{\sqrt{\sum_d x_d^2}}$$

Unit Vector



Linear Regression

[Image: Murphy, K. (2012)]



For D-dimensional input vector $x \in \mathbb{R}^D$ the plane equation,

$$y = w^T x + b$$

Sometimes we simplify this by including the intercept into the weight vector,

$$\widetilde{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_D \\ b \end{pmatrix} \qquad \widetilde{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_D \\ 1 \end{pmatrix} \qquad y = \widetilde{w}^T \widetilde{x}$$

Since:

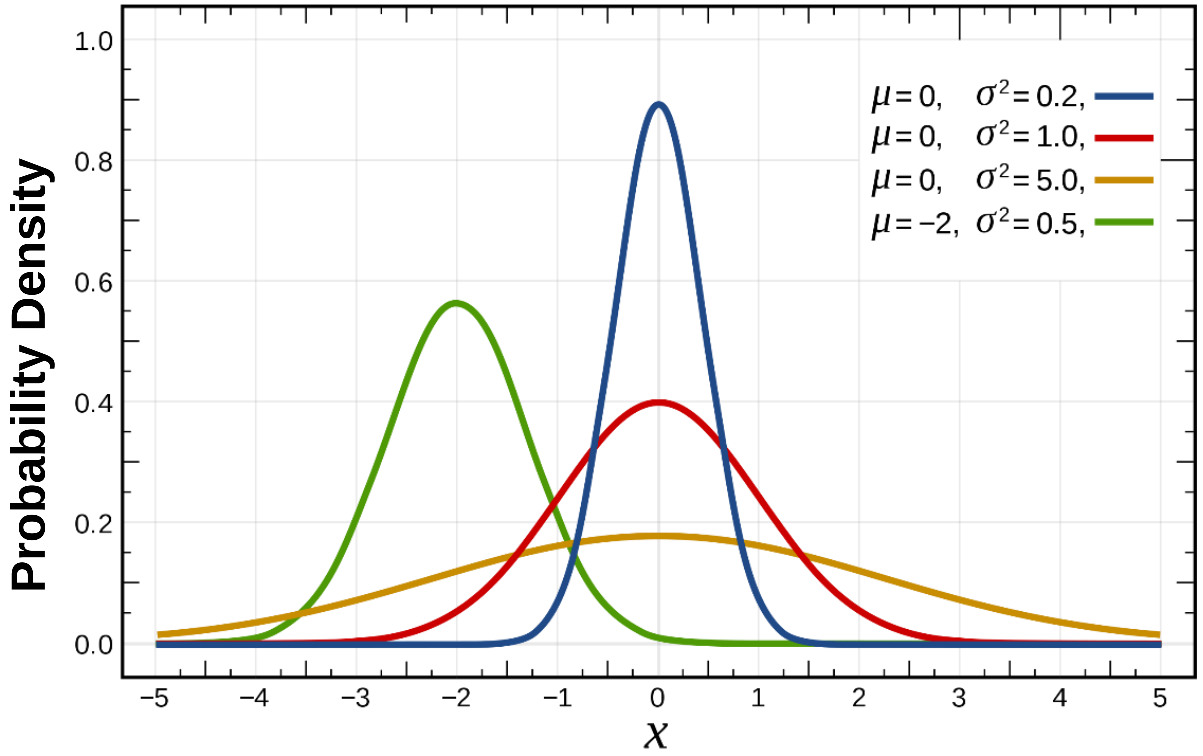
$$\widetilde{w}^T \widetilde{x} = \sum_{d=1}^{D} w_d x_d + b \cdot 1$$
$$= w^T x + b$$

Modeling Noise in Data

Gaussian (a.k.a. Normal) distribution with mean (location) μ and variance (scale) σ^2 parameters,

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{1}{2}(x-\mu)^2/\sigma^2$$

We say $X \sim \mathcal{N}(X \mid \mu, \sigma^2)$



Useful Properties

- Closed under independent addition:

$X \sim \mathcal{N}(\mu_x, \sigma_x^2) \qquad Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$ X, Y indepdent

$$X + Y \sim \mathcal{N}(\mu_x + \mu_y, \sigma_x^2 + \sigma_y^2)$$

- Closed under linear transformation (a and b constant):

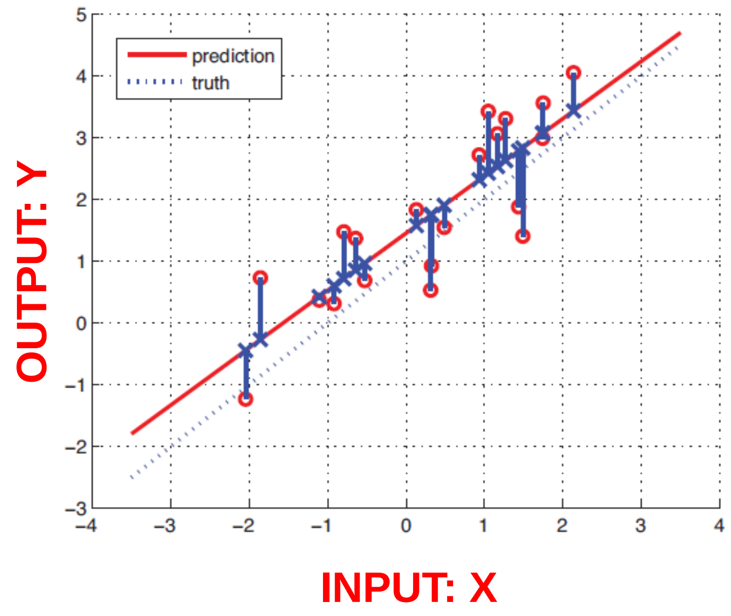
$$aX + b \sim \mathcal{N}(a\mu_x + b, a^2\sigma_x^2)$$

Linear Regression

Input-output mapping is not exact, so we will assume data has zero-mean Gaussian noise,

Multivariate Normal (uncorrelated)

$$y = w^T x + \epsilon \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$



This is equivalent to:

$$p(y \mid w, x) = \mathcal{N}(y \mid w^T x, \sigma^2)$$

Because Adding a constant to a Normal RV is still a Normal RV,

$$z \sim \mathcal{N}(m, P) \qquad z + c \sim \mathcal{N}(m + c, P)$$

In the case of linear regression $z \rightarrow \epsilon$ and $c \rightarrow w^T x$

Learning linear regression models

We need to learn the model from data
by learning the regression weights

Data – We have this

$$y = w^T x + \epsilon$$

Random; Can't do anything about it

Don't know these; need to learn them

How to do this?
What makes *good* weights?

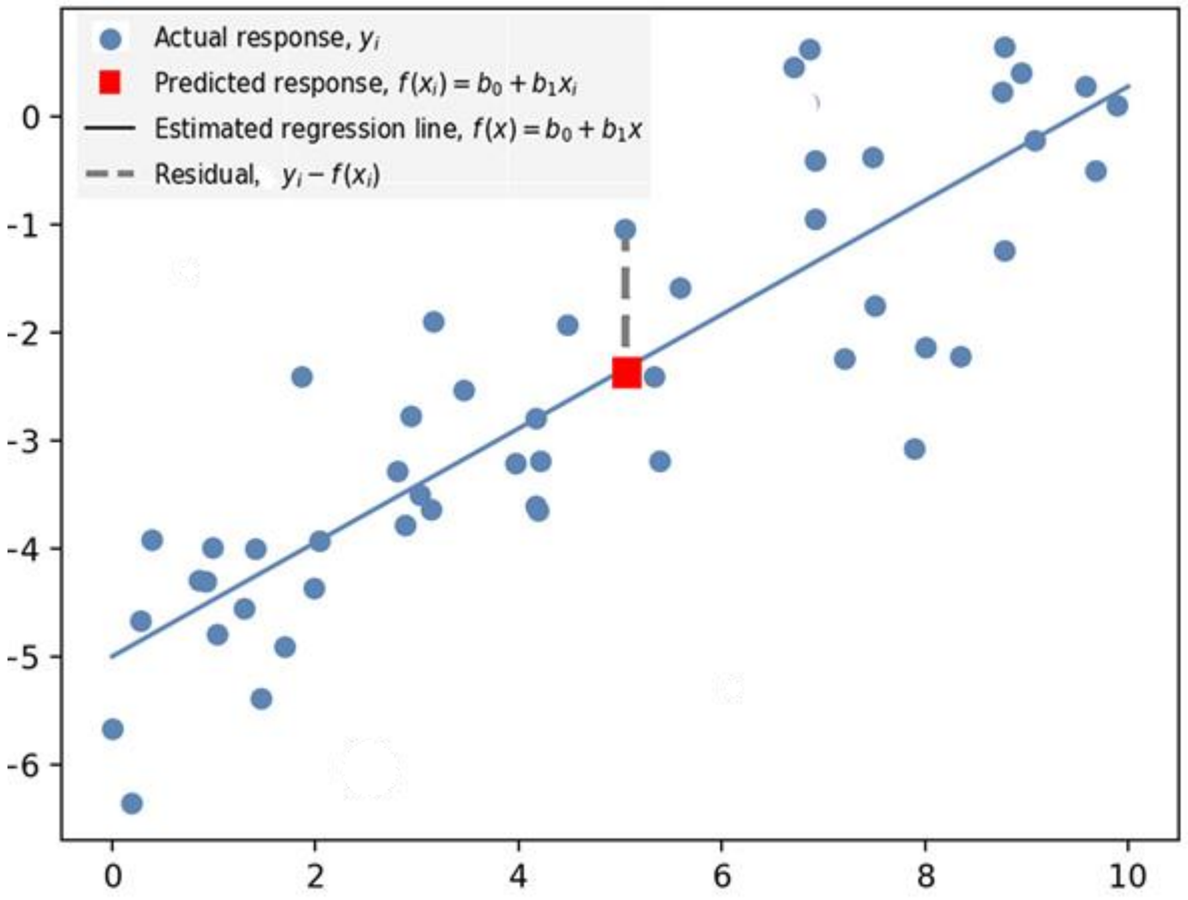
Learning Linear Regression Models

There are several ways to think about fitting regression:

- **Intuitive** Find a plane/line that is close to data
- **Functional** Find a line that minimizes the *least squares* loss
- **Estimation** Find maximum likelihood estimate of parameters

They are all equivalent…

Fitting Linear Regression



Intuition Find a line that is as *close as possible* to every training data point

The distance from each point to the line is the **residual**

$$y - w^T x$$

https://www.activestate.com/resources/quick-reads/how-to-run-linear-regressions-in-python-scikit-learn/

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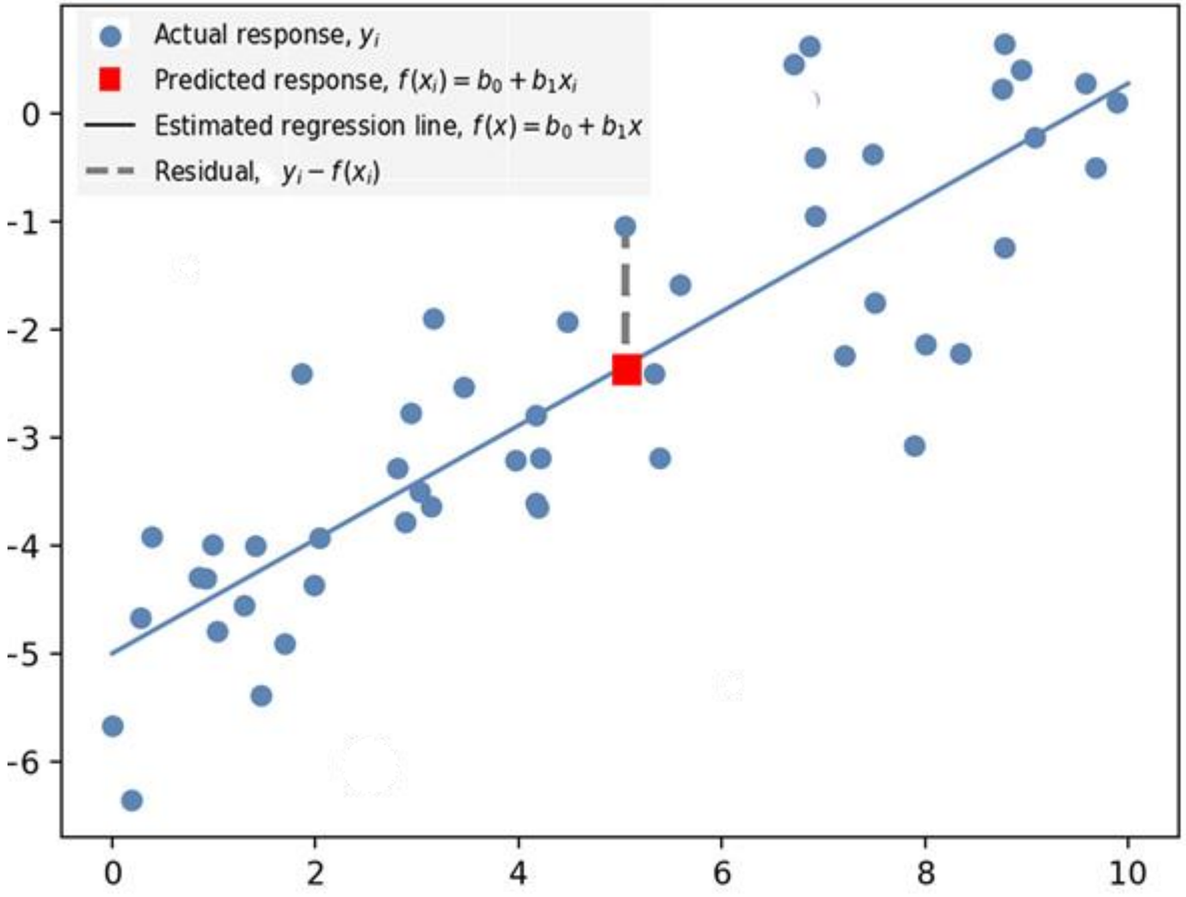
Least Squares Solution



Functional Find a line that minimizes the sum of squared residuals

$$w^* = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

Over all the training data,

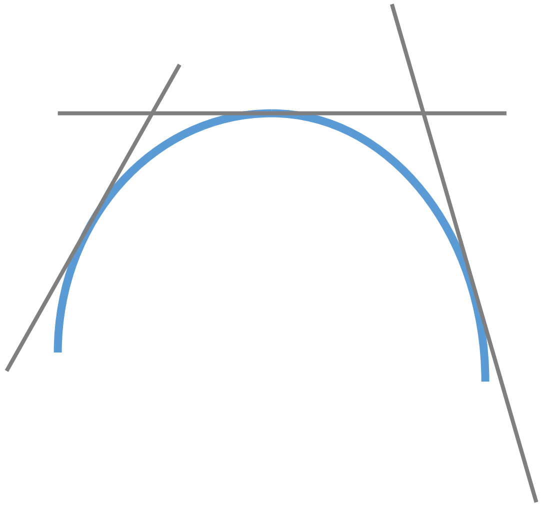
$$\{(x_i, y_i)\}_{i=1}^{N}$$

Least squares regression

https://www.activestate.com/resources/quick-reads/how-to-run-linear-regressions-in-python-scikit-learn/

Optimization basics

Example: maximize $f(\theta) = -a\theta^2 + b\theta + c$ with $a > 0$



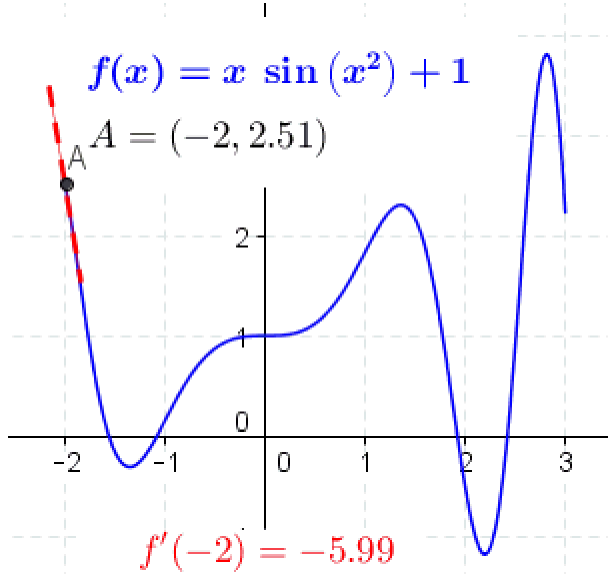
It is a quadratic function.
=> finding the 'flat' point suffices

Compute the gradient and set it equal to 0 (stationary points)

$$f'(\theta) = -2a\theta + b \quad \Rightarrow \quad \theta = \frac{b}{2a}$$

Closed form!

Q: Does this trick of grad=0 work for other functions?
$\Rightarrow$ Yes for maximization of **<u>concave</u>** functions
or minimization of **<u>convex</u>** functions



(gradient illustration)

- [Def] A set C is convex if

$$\forall u, v \in C, \forall \alpha \in [0,1], \text{ we have } \alpha u + (1-\alpha)v \in C$$

convex combination
Line segment between u, v

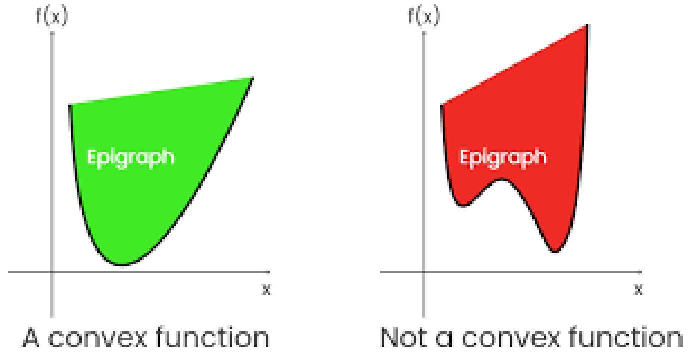
Convex function: intuition

- **<u>Informally</u>**,
  - A convex function is one that looks “convex” from the bottom
  - A convex function has only one “valley”

Convex functions

Nonconvex function

  - A convex function is one whose epigraph is a convex set

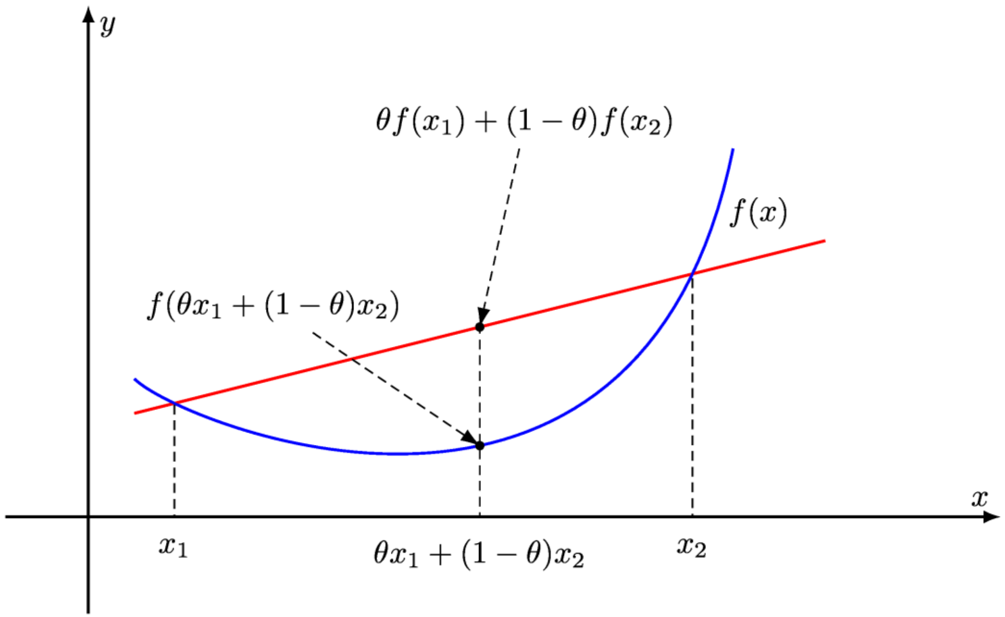


Convex function: formal definition

- **Formally,**

  [Def] Let C be a convex set. A function $f: C \to \mathbb{R}$ is convex if $\forall u, v \in C$ and $\forall \alpha \in [0,1]$,

$$f(\alpha u + (1-\alpha)v) \le \alpha f(u) + (1-\alpha) f(v)$$



- [Def] Function f is said to be concave, if $-f$ is convex

Optimization basics

What if there is no closed form solution?

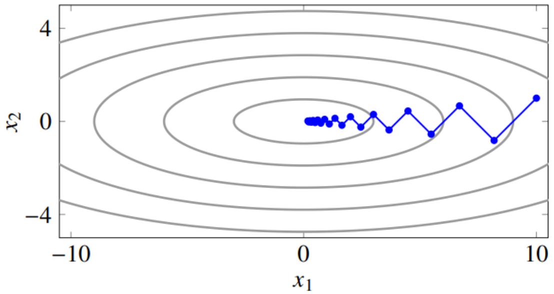
Example: $f(\theta) = \frac{1}{2}x(ax - 2\log(x) + 2)$

$$f'(\theta) = ax - \log(x)$$

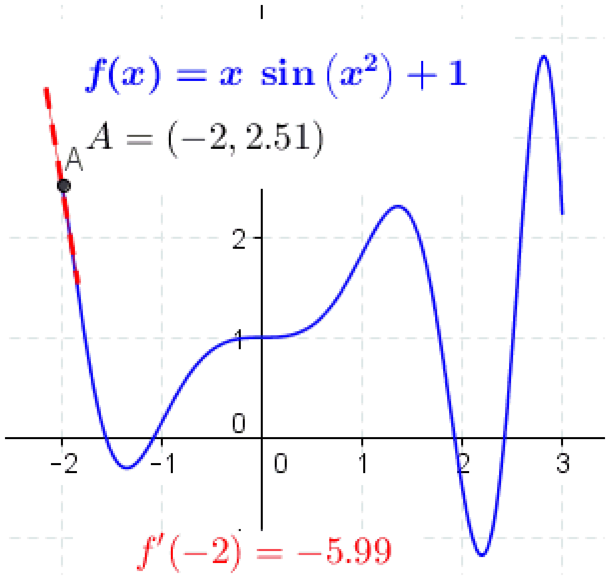
No known closed form for $ax = \log(x)$

Iterative methods:

- Hillclimbing - gradient descent
- Newton's method
- Etc.



Iterative methods for optimization
=> Will find the global minimum
for **convex** functions (convex optimization)
⇒ More generally, finds a local minimum but could also get stuck at *stationary points*.



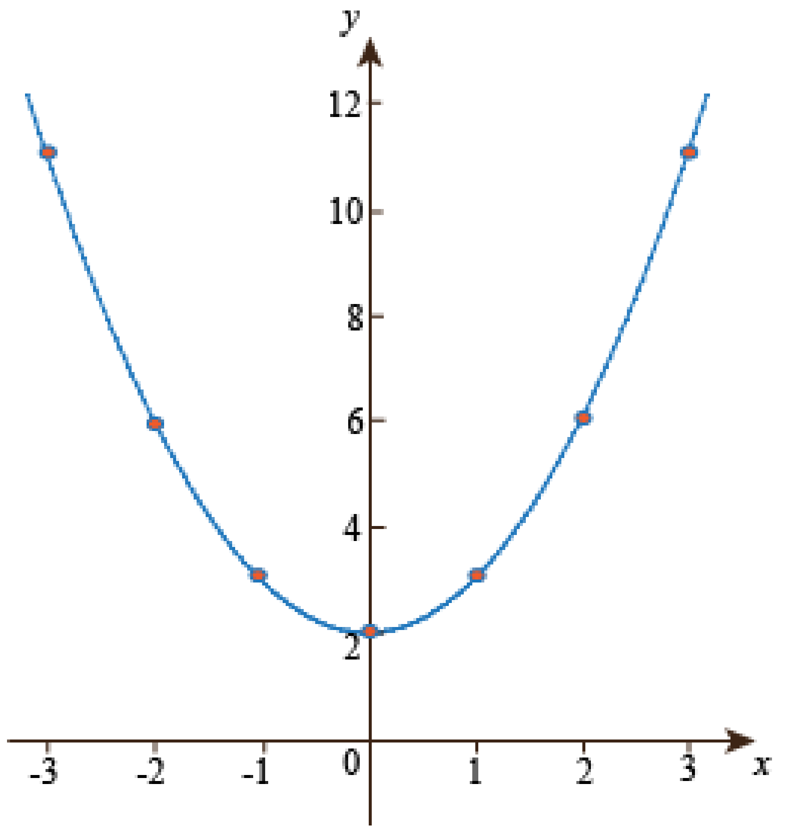
Q: find the stationary points and global minimum

Least Squares

$$\min_{w} \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

This is just a quadratic function…

- *Convex* => all local minima are global
- Minimum given by zero-derivative
- Can find a closed-form solution



Let’s see for scalar case with no bias,

$$y = wx$$

Least Squares : Simple Case

$$\frac{d}{dw}\sum_{i=1}^{N}(y_i - wx_i)^2 =$$

Derivative (+ chain rule)

$$= \sum_{i=1}^{N} 2(y_i - wx_i)(-x_i) = 0 \Rightarrow$$

Distributive Property

$$0 = \sum_{i=1}^{N} y_i x_i - w\sum_{j=1}^{N} x_j^2$$

Algebra

$$w = \frac{\sum_i y_i x_i}{\sum_j x_j^2}$$

Least Squares in Higher Dimensions

Things are a bit more complicated in higher dimensions and involve more linear algebra,

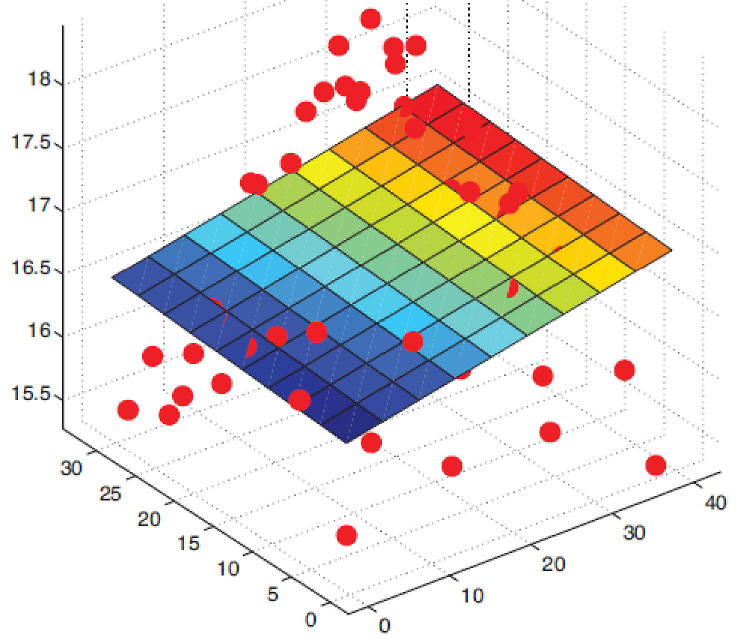
$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1D} \\ 1 & x_{21} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & \dots & x_{ND} \end{pmatrix}$$

Design Matrix
(each training input on a row)

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$$

Vector of
Training labels

[Image: Murphy, K. (2012)]



Can write regression over *all training data* more compactly…

$$\mathbf{y} = \mathbf{X}w$$

Nx1 Vector

Least Squares in Higher Dimensions

Least squares can also be written more compactly,

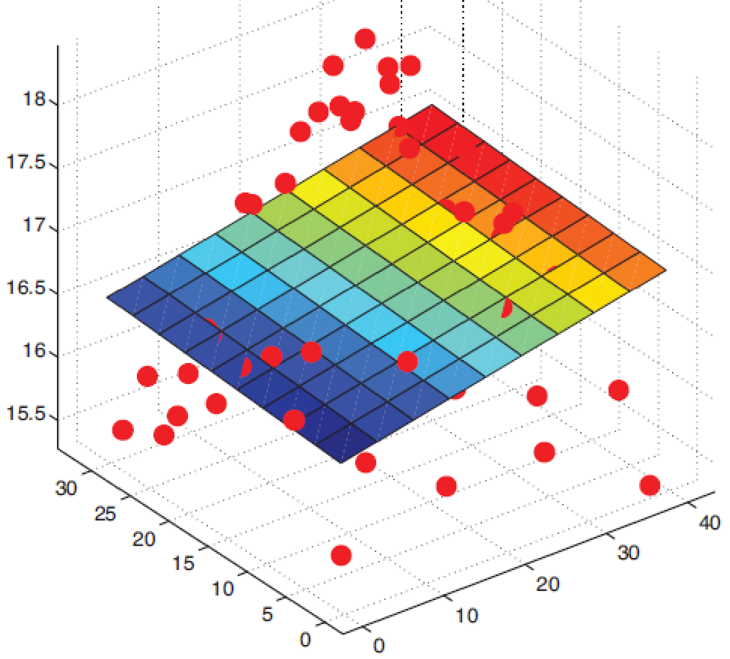
$$\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 = \|\mathbf{y} - \mathbf{X}w\|^2$$

Some slightly more advanced linear algebra gives us a solution,

$$w = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Ordinary Least Squares (OLS) solution

[Image: Murphy, K. (2012)]



Derivation a bit involved for lecture but…
- We know it has a closed-form and why
- We can evaluate it
- Generally know where it comes from

Learning Linear Regression Models

There are several ways to think about fitting regression:

- **Intuitive** Find a plane/line that is close to data
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They are all the same thing…

Learning Linear Regression Models

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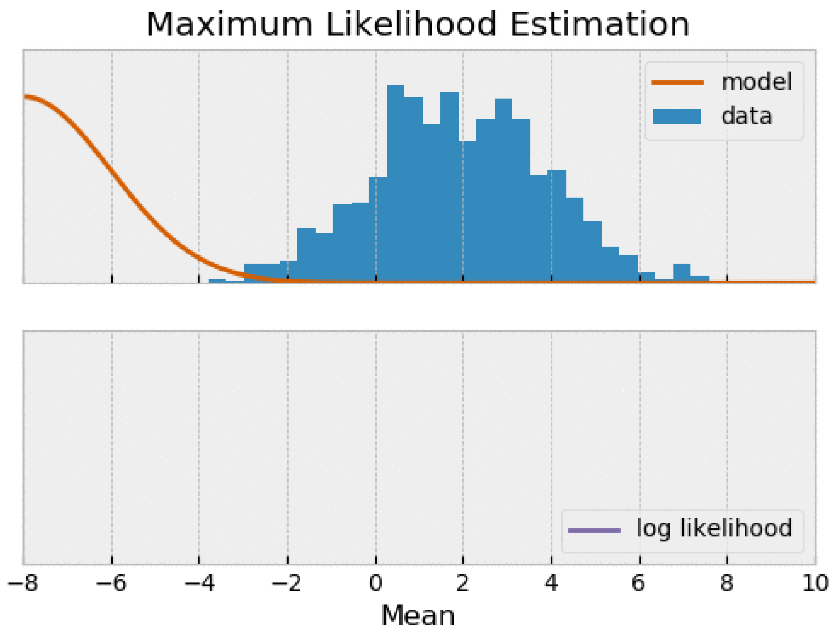
Recap: Maximum Likelihood Estimation

Suppose we observe N data points from a Gaussian model $\mathcal{N}(\mu, \sigma^2)$ and wish to estimate its mean parameter μ



Likelihood Principle: *Given a statistical model, the <u>likelihood function</u> describes how well a parameter "supports" the observed data (evidence)*

https://towardsdatascience.com/maximum-likelihood-estimation-984af2dcfcac

Recap: MLE of Gaussian Mean

Assume data are i.i.d. univariate Gaussian,

Variance is known

$$p(\mathcal{Y} \mid \mu) = \prod_{i=1}^{N} \mathcal{N}(y_i \mid \mu, \sigma^2)$$

Log-likelihood function:

$$\mathcal{L}(\mu) = \sum_{i=1}^{N} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}(y_i - \mu)^2 \sigma^{-2}\right)\right)$$

Constant doesn't depend on mean

$$= \text{const.} - \frac{1}{2}\sum_{i=1}^{N}\left((y_i - \mu)^2 \sigma^{-2}\right)$$

MLE doesn't change when we:
1) Drop constant terms (in μ)
2) Minimize negative log-likelihood

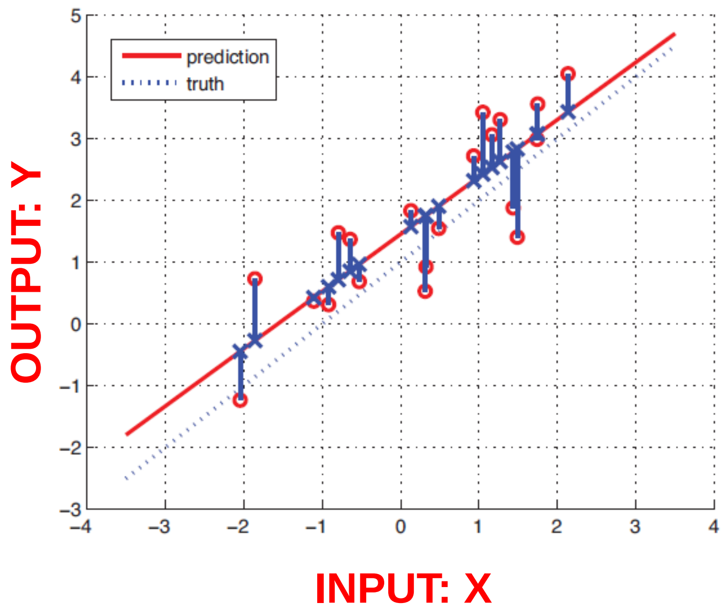
MLE estimate is *least squares estimator*:

$$\mu^{\text{MLE}} = \arg\max_{\mu} -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \mu)^2 = \arg\min_{\mu} \sum_{i=1}^{N}(y_i - \mu)^2$$

MLE for Linear Regression

Given training data $\{(x_i, y_i)\}_{i=1}^N$ likelihood function is given by,

$$\log \prod_{i=1}^N p(y_i \mid x_i, w) = \sum_{i=1}^N \log p(y_i \mid x_i, w)$$



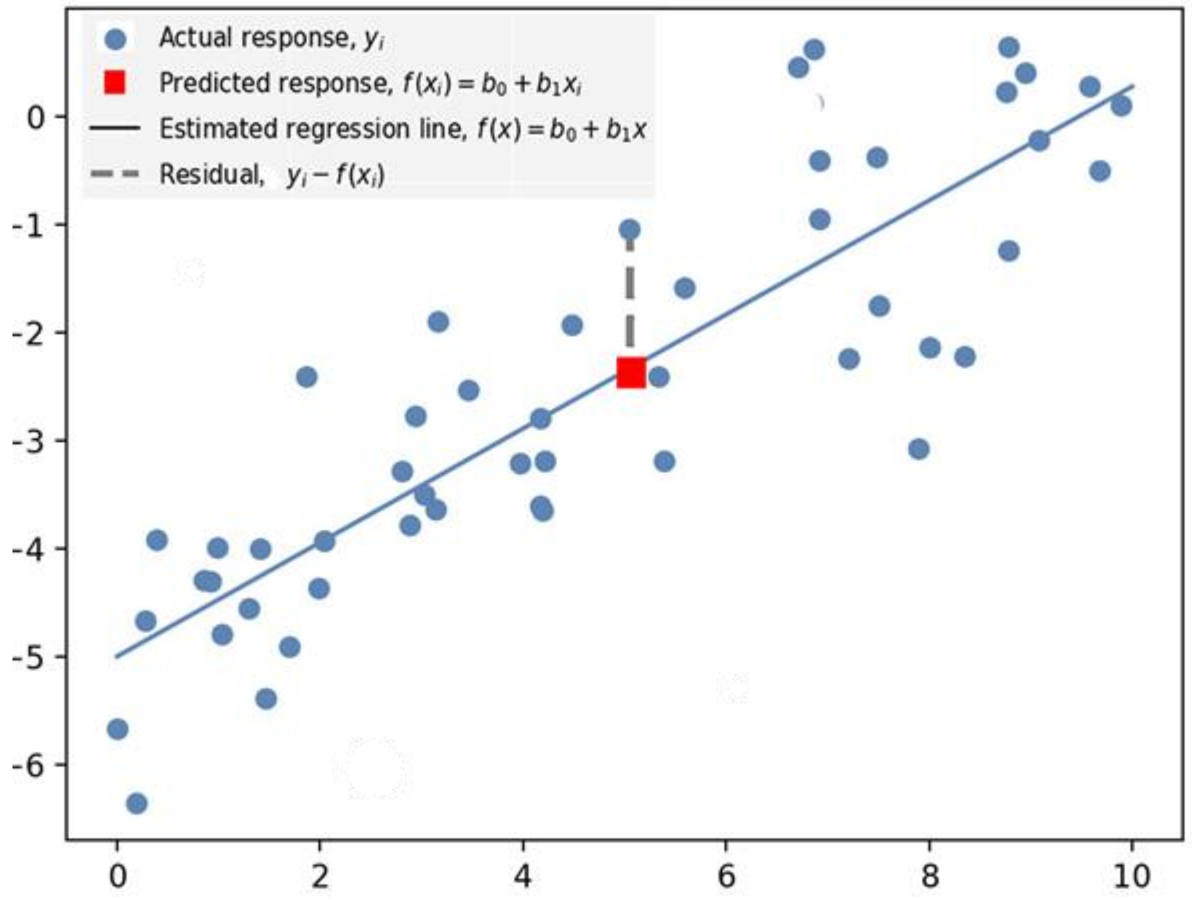
Recall that the likelihood is Gaussian:

$$p(y \mid w, x) = \mathcal{N}(y \mid w^T x, \sigma^2)$$

So MLE maximizes the log-likelihood over the whole data as,

$$w^{\text{MLE}} = \arg\max_w \sum_{i=1}^N \log \mathcal{N}(y_i \mid w^T x_i, \sigma^2) = \arg\max_w \sum_{i=1}^N \text{const} - \frac{1}{2\sigma^2}(y_i - w^T x_i)^2$$

MLE for Linear Regression



After simplification, we have,

$$w^{\text{MLE}} = \min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

So for Linear Regression, MLE = Least Squares Estimation

https://www.activestate.com/resources/quick-reads/how-to-run-linear-regressions-in-python-scikit-learn/

MLE for Linear Regression

Using previous results, MLE is equivalent to minimizing squared residuals,

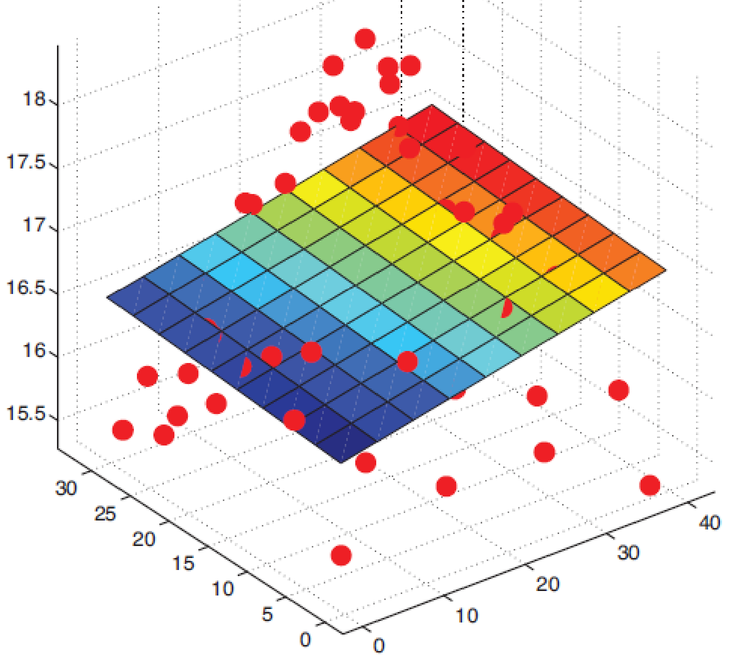
$$\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 = \|\mathbf{y} - \mathbf{X}w\|^2$$

Some slightly more advanced linear algebra gives us a solution,

$$w = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Ordinary Least Squares (OLS) solution

[Image: Murphy, K. (2012)]



Derivation a bit involved for lecture but…

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Linear Regression Summary

1. Definition of linear regression model,

$$y = w^T x + \epsilon \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

2. For N iid training data fit using least squares,

$$w^{\text{OLS}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

3. Equivalent to maximum likelihood solution

Linear Regression Summary

Ordinary least squares solution

$$w^{\text{OLS}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

Is solved in closed-form using the Normal equations,

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1D} \\ 1 & x_{21} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & \dots & x_{ND} \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \qquad w^{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Design Matrix
(each training input on a column)

Vector of
Training labels

A word on matrix inverses…

$$w^{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Least squares solution requires inversion of the term,

$$(\mathbf{X}^T\mathbf{X})^{-1}$$

What are some issues with this?

1. Requires $\mathcal{O}(D^3)$ time for D input features

2. May be numerically unstable (or even non-invertible)

$$(x+\epsilon)^{-1} = \frac{1}{x+\epsilon}$$

→ **Small numerical errors in input can lead to large errors in solution**

Pseudoinverse

The *Moore-Penrose pseudoinverse* is denoted as X^{+}

$$w^{\mathrm{OLS}} = X^{+}y$$

- Generalization of the standard matrix inverse
  - If $X^{\top}X$ is invertible, $X^{+} = (X^{\top}X)^{-1}X^{\top}$
- Exists even for non-invertible $X^{T}X$
- Directly computable in most libraries
- In Numpy it is: `linalg.pinv`

Linear Regression in Scikit-Learn

Load your libraries,

For Evaluation

```
import matplotlib.pyplot as plt
import numpy as np
from sklearn import datasets, linear_model
from sklearn.metrics import mean_squared_error, r2_score
```

Load data,

```
# Load the diabetes dataset
diabetes_X, diabetes_y = datasets.load_diabetes(return_X_y=True)

# Use only one feature
diabetes_X = diabetes_X[:, np.newaxis, 2]
```

Samples total	442
Dimensionality	10
Features	real, -.2 < x < .2
Targets	integer 25 - 346

Train / Test Split:

```
diabetes_X_train = diabetes_X[:-20]
diabetes_X_test = diabetes_X[-20:]
```

```
diabetes_y_train = diabetes_y[:-20]
diabetes_y_test = diabetes_y[-20:]
```

Linear Regression in Scikit-Learn

Train (fit) and predict,

```python
# Create linear regression object
regr = linear_model.LinearRegression()

# Train the model using the training sets
regr.fit(diabetes_X_train, diabetes_y_train)

# Make predictions using the testing set
diabetes_y_pred = regr.predict(diabetes_X_test)
```

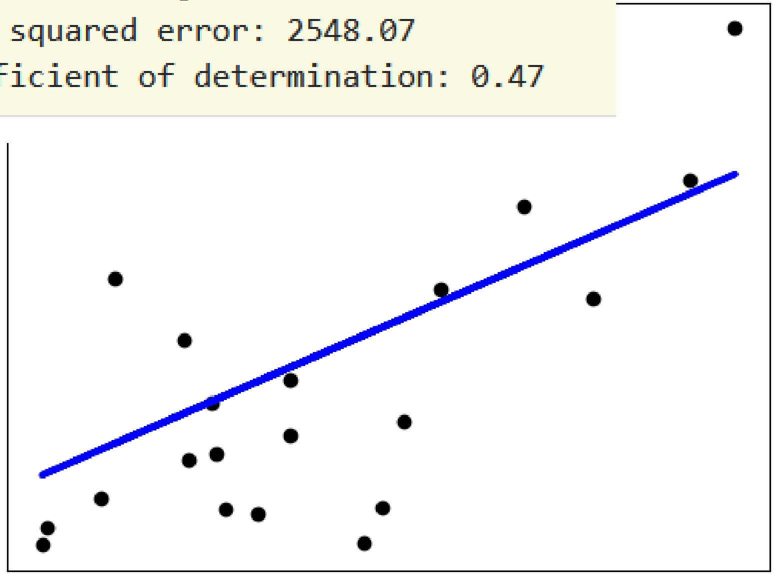
Plot regression line with the test set,

```python
# Plot outputs
plt.scatter(diabetes_X_test, diabetes_y_test, color="black")
plt.plot(diabetes_X_test, diabetes_y_pred, color="blue", linewidth=3)

plt.xticks(())
plt.yticks(())

plt.show()
```

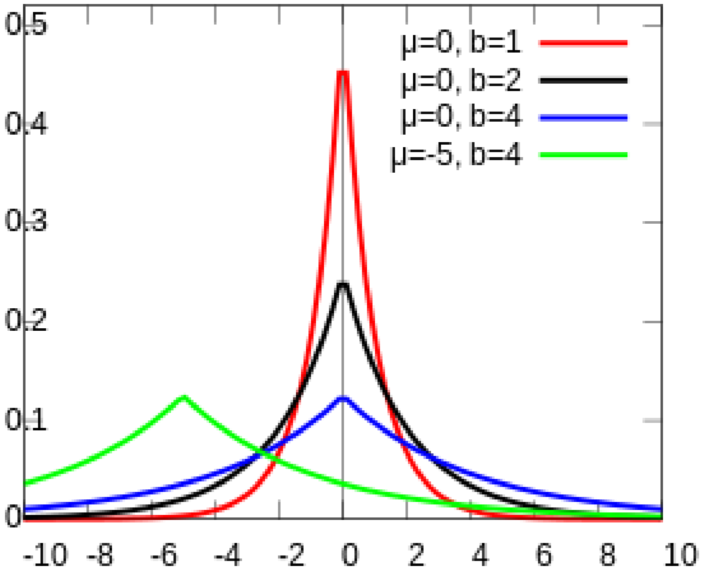
```
Coefficients:
 [938.23786125]
Mean squared error: 2548.07
Coefficient of determination: 0.47
```



Linear regression: extensions

- What if we have multivariate label $y \in \mathbb{R}^k$?
  - Conceptually, can think about the prediction from x to y as k separate linear regression problems

- How to compute MLE if the model is $y = w^T x + \epsilon$, $\epsilon \sim$ other distributions beyond Gaussian?
  - E.g. ϵ is drawn from Laplace(0,1)
  - (Exercise)



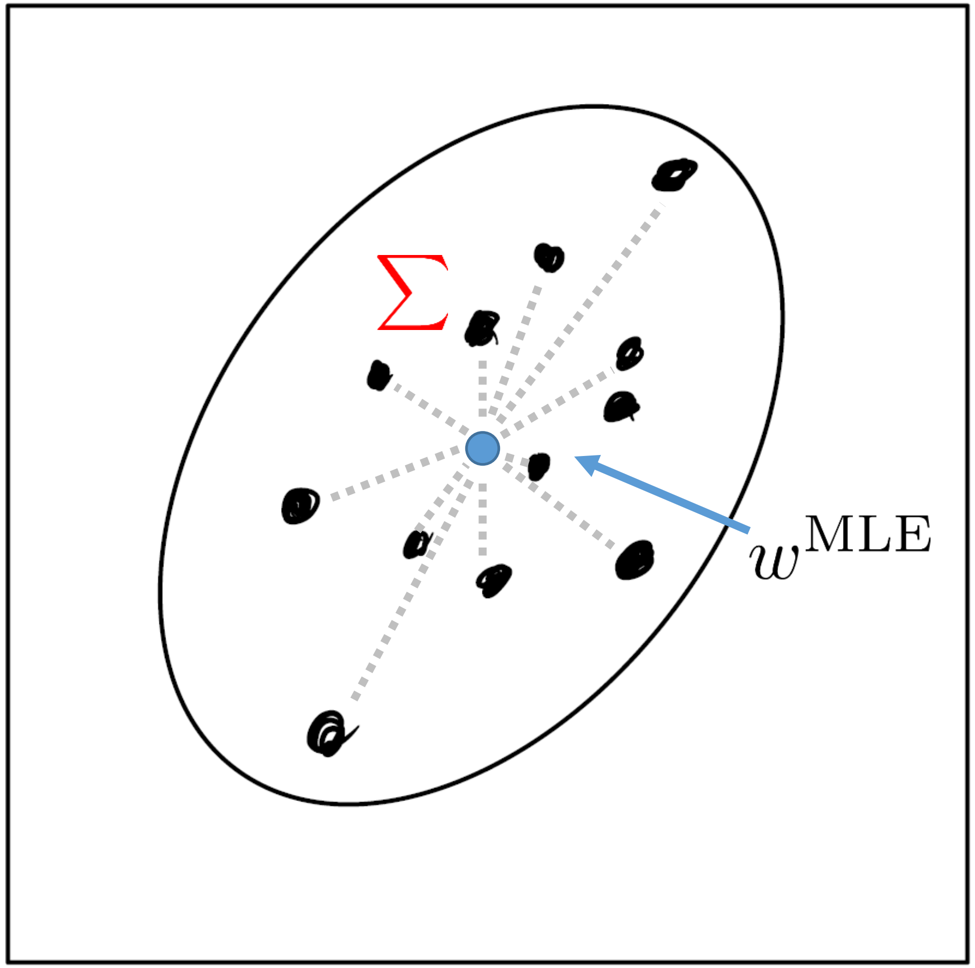
Outline

- Linear Models for Regression
  - Least Squares Estimation
  - Regularized Least Squares
- Linear Models for Classification
  - Logistic Regression
  - Support Vector Machine

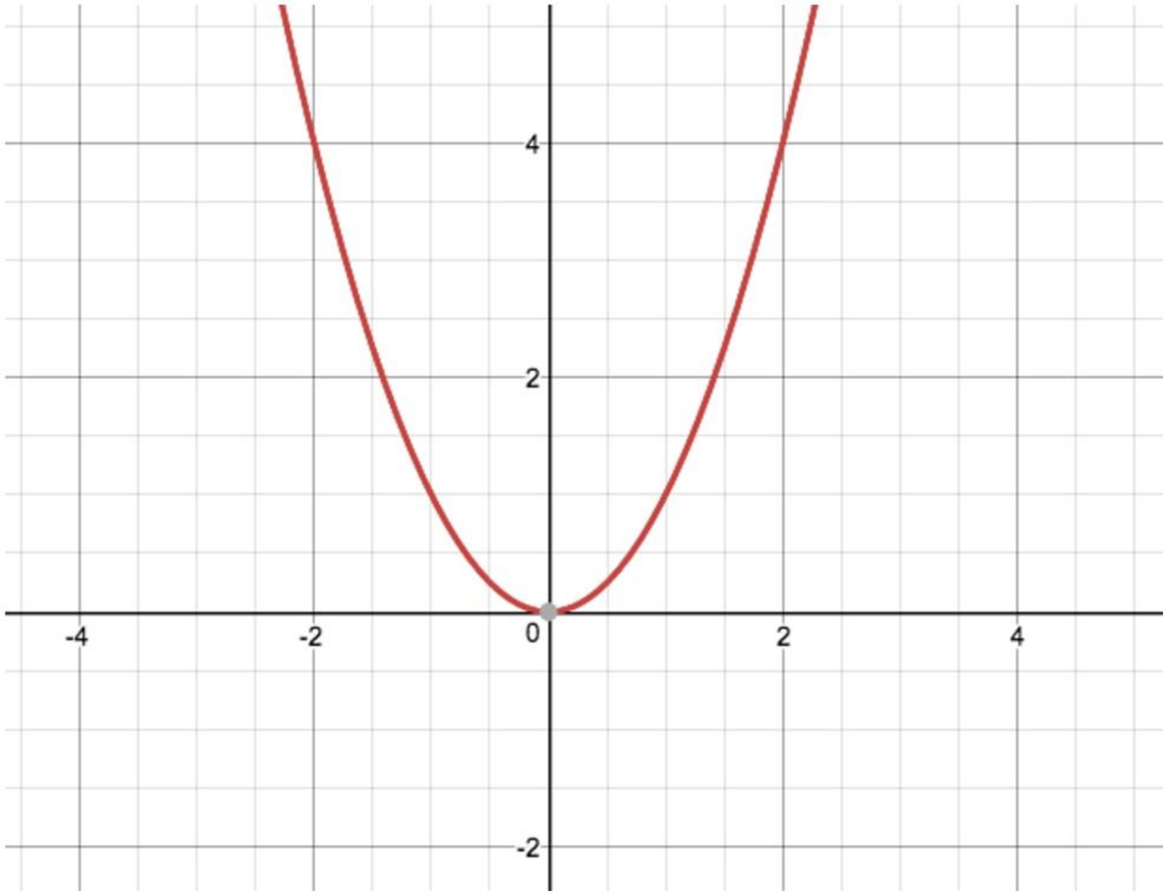
Outliers

How does an outlier affect the estimator?

Example: estimate the mean of a population



Squared Error



Outliers

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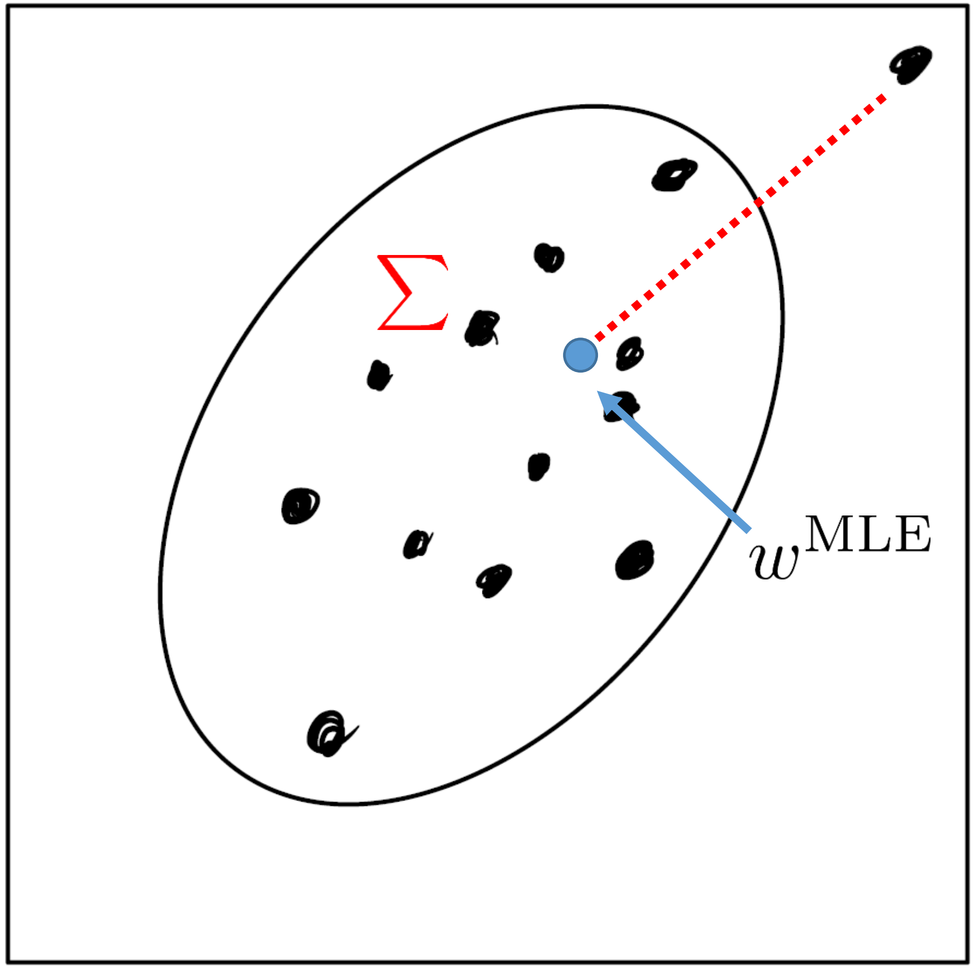
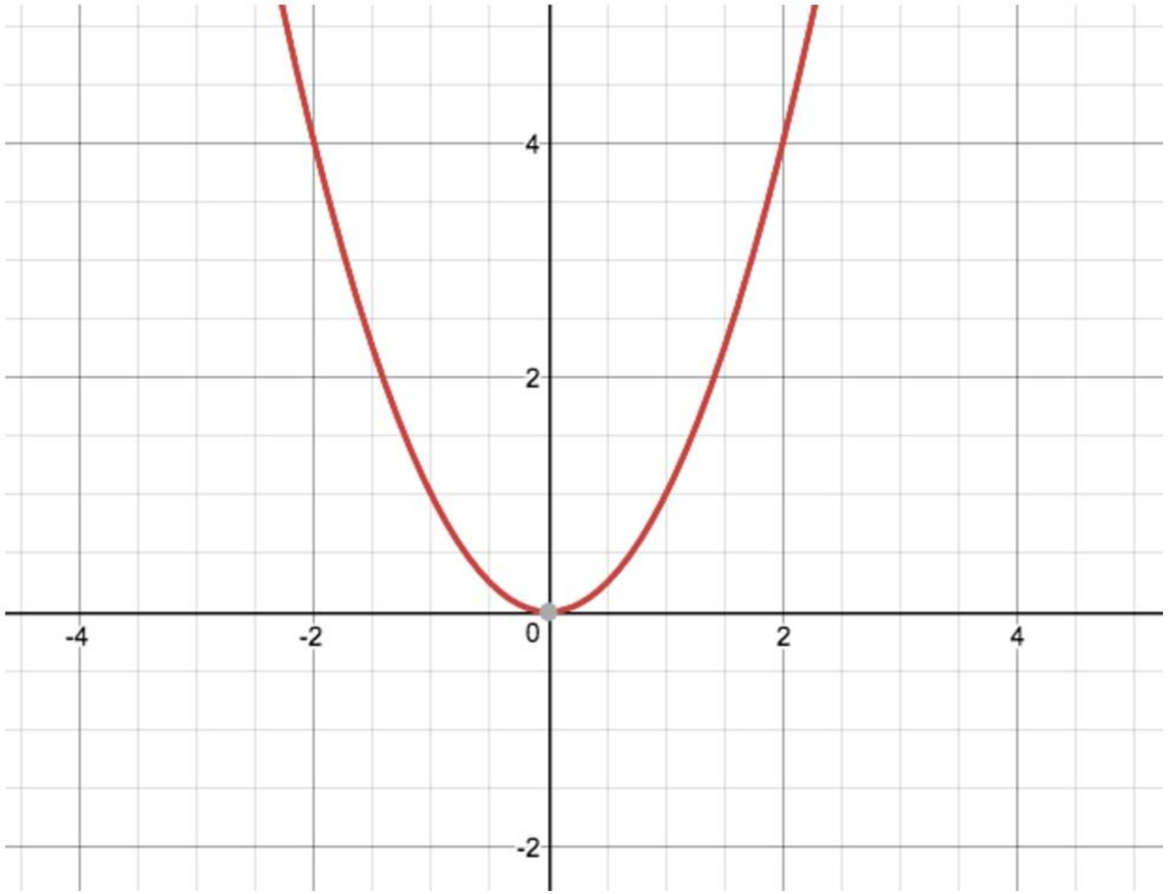
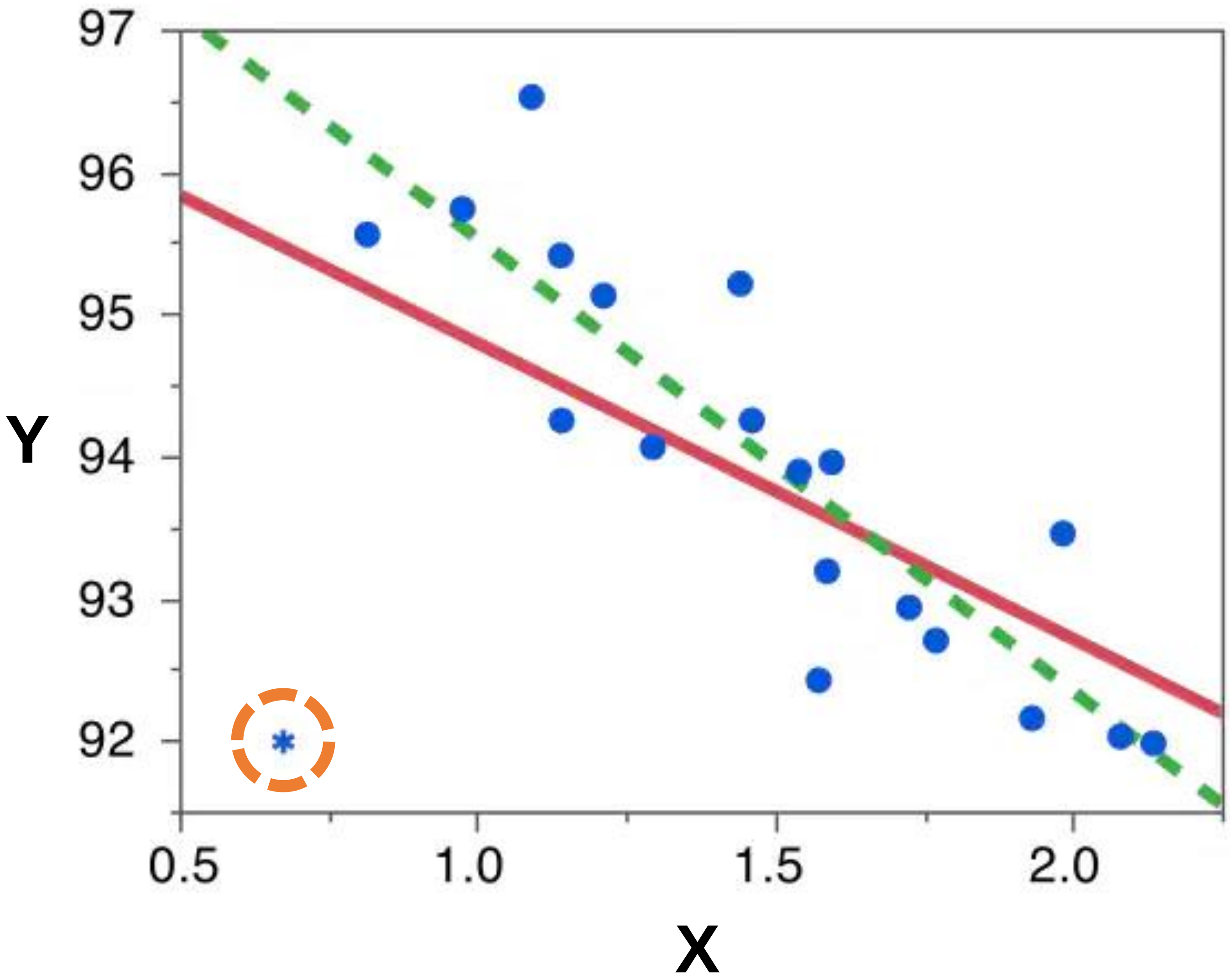


Squared Error



Outliers in Linear Regression



Outlier "pulls" regression line away from inlier data

Need a way to *ignore* or to *down-weight* impact of outlier

https://www.jmp.com/en_us/statistics-knowledge-portal/what-is-multiple-regression/mlr-residual-analysis-and-outliers.html

Dealing with Outliers

Too many outliers can indicate many things: non-Gaussian (heavy-tailed) data, corrupted data, bad data collection, …

A few ways to handle outliers…

1. Use a heavy-tailed distribution to model noise (e.g. Student's t)

Fitting regression becomes difficult

2. Identify outliers and discard them

Perhaps needs to solve a NP-Hard problem & throwing away data is generally bad

3. Penalize extreme weights to avoid overfitting (Regularization)

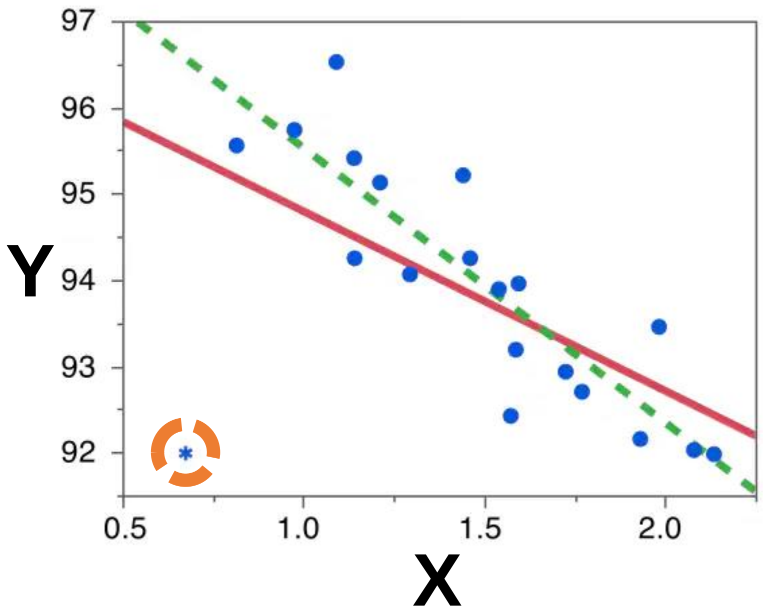
Regularization

Regularization helps avoid overfitting to training data…

$$\text{Model} = \min_{\text{model}} \text{Loss}(\text{Model}, \text{Data}) + \lambda \cdot \text{Regularizer}(\text{Model})$$

Regularization Strength

Regularization Penalty



Red model is without regularization

Green model is with regularization

Regularized Least Squares

A couple regularizers are so common they have specific names

L2 Regularized Linear Regression

- Ridge Regression
- aka Tikhonov Regularization

L1 Regularized Linear Regression

- LASSO
- Stands for “Least Absolute Shrinkage and Selection Operator”

Regularized Least Squares

Ordinary least-squares estimation (no regularizer),

Already know how to solve this…

$$w^{\mathrm{OLS}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

L2-regularized Least-Squares (Ridge)

Quadratic Penalty

$$w^{\mathrm{L2}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \frac{\lambda}{2}\|w\|^2$$

L1-regularized Least-Squares (LASSO)

Absolute Value (L1) Penalty

$$w^{\mathrm{L1}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \lambda|w|$$

A word on vector norms…

The *L2-norm* (Euclidean norm) of a vector w is,

$$\|w\| = \sqrt{w^T w} = \sqrt{\sum_{d=1}^{D} w_d^2} \qquad \|w\|^2 = \sum_{d=1}^{D} w_d^2$$

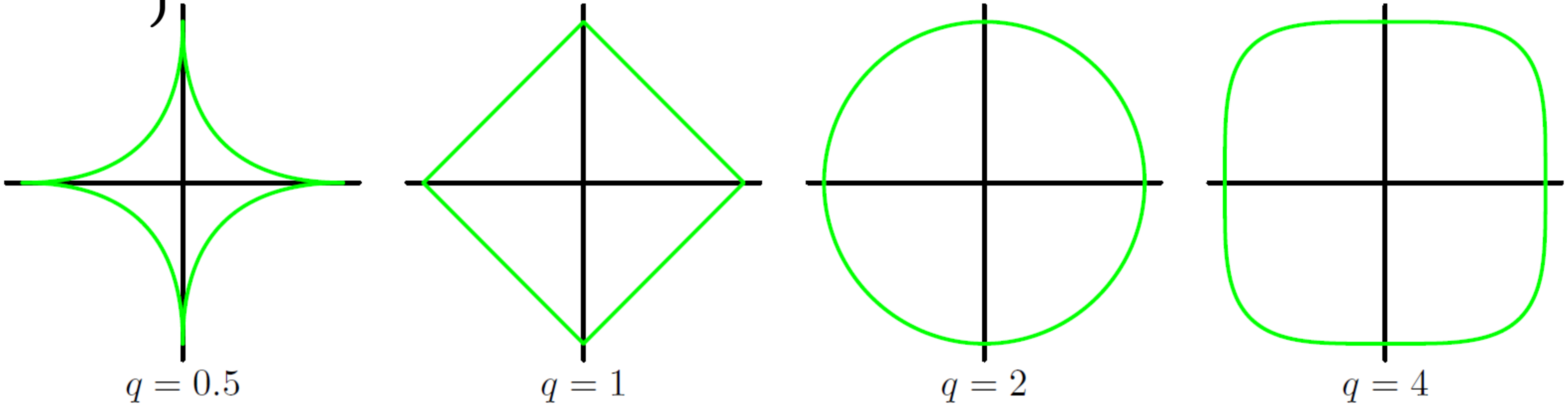
The *L1-norm* (absolute value) of a vector w is,

$$|w| = \sum_{d=1}^{D} |w_d|$$

They are not the same functions…

Other Regularization Terms

$$\left\{ w : \sum_{i=1}^{d} |w_i|^q \leq 1 \right\}$$



q<1 is not a norm, and thus not convex

L1 is non-differentiable

L2 Regularization

A more general regularization penalty:

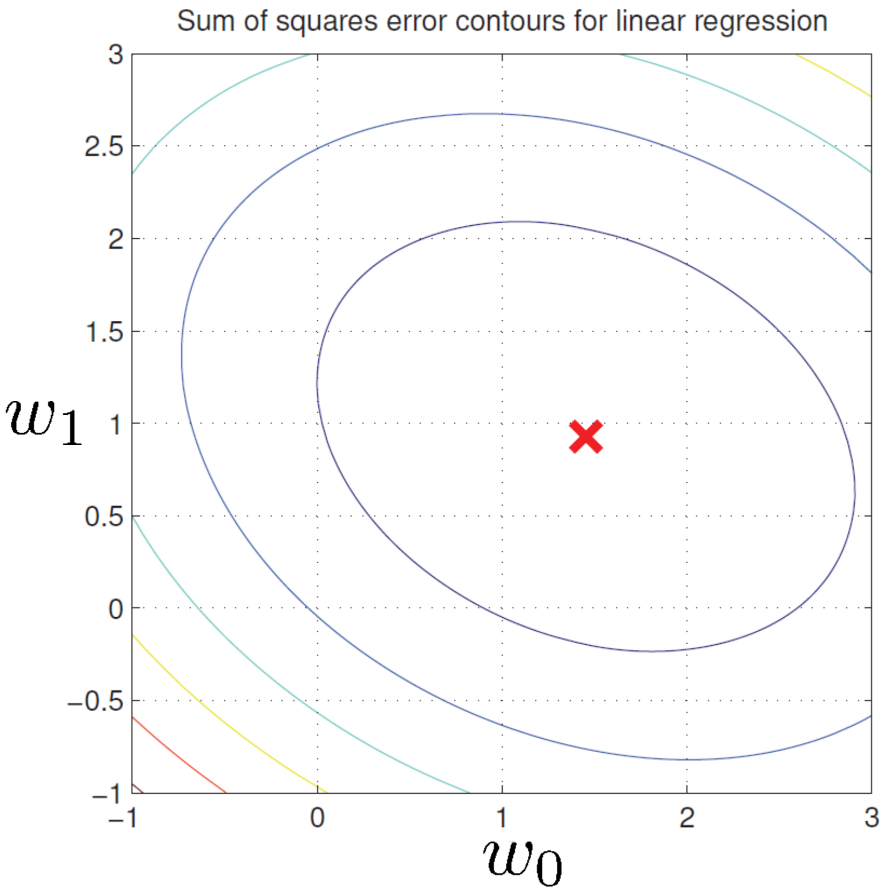
$$\hat{w} = \arg\min_{w} \frac{1}{2} \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \frac{\lambda}{2} \sum_{i=1}^{d} |w_i|^q$$

L2 Regularized Least Squares

$$w^{\mathrm{L2}} = \arg\min_{w} \underbrace{\sum_{i=1}^{N} (y_i - w^T x_i)^2}_{\text{Quadratic}} + \overbrace{\frac{\lambda}{2}\|w\|^2}^{\text{Quadratic}}$$

Quadratic + Quadratic = Quadratic

- Differentiable
- Convex
- Unique optimum
- Closed form solution



L2 Regularized Least Squares : Simple Case

$$\frac{d}{dw}\frac{1}{2}\sum_{i=1}^{N}(y_i - wx_i)^2 + \frac{\lambda}{2}\frac{d}{dw}w^2 =$$

Derivative (+ chain rule)

$$= \sum_{i=1}^{N}(y_i - wx_i)(-x_i) + \lambda w \quad = 0 \Rightarrow$$

Distributive Property

$$0 = \sum_{i=1}^{N} y_i x_i - w\sum_{j=1}^{N} x_j^2 - \lambda w$$

Algebra

$$w = \frac{\sum_i y_i x_i}{\lambda + \sum_j x_j^2}$$

L2 Regularized Linear Regression – Ridge Regression

Source: Kevin Murphy's Textbook

$$w^{\mathrm{L2}} = \arg\min_{w} \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \frac{\lambda}{2} \|w\|^2$$

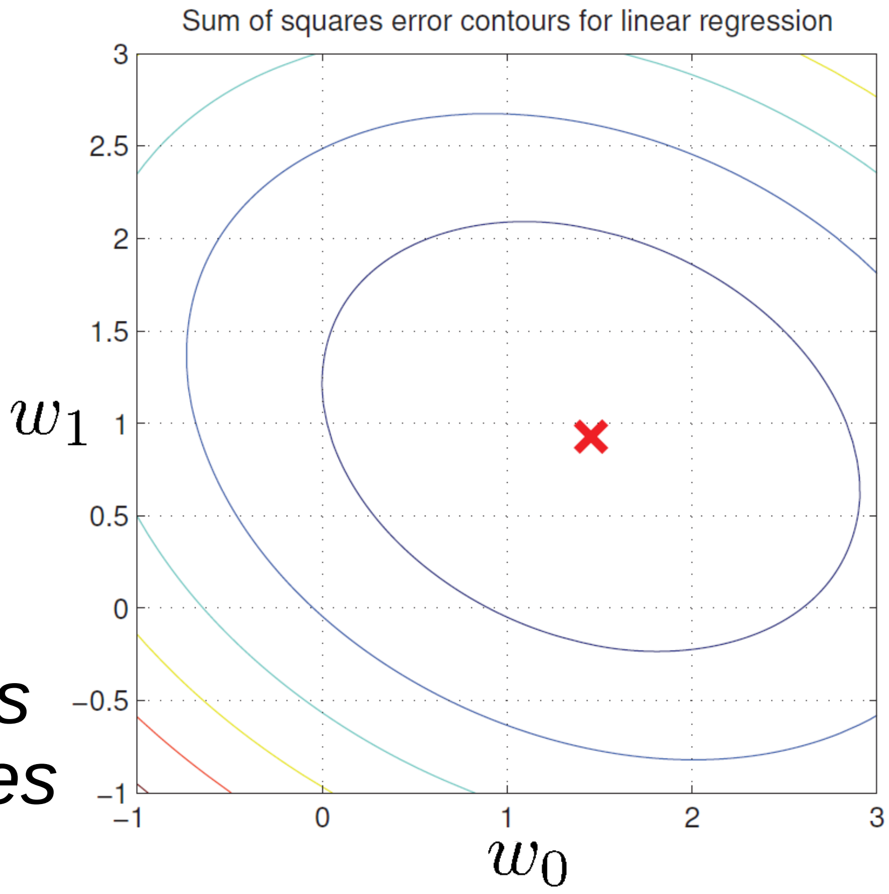
After some algebra…

$$w^{\mathrm{L2}} = (\lambda I + \mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Compare to ordinary least squares:

$$w^{\mathrm{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Regularized least-squares can be viewed as OLS with additional pseudo-training examples



Notes on L2 Regularization

- Feature weights are "shrunk" towards zero (and each other) – statisticians often call this a "shrinkage" method
- Typically do **not** penalize bias (y-intercept, w_0) parameter,

$$\min_w \sum_i (y_i - w^T x_i - w_0)^2 + \lambda \sum_{d=1}^{D} w_d^2$$

- This way the solution will be invariant to data shifting

- Solutions are **not** invariant to scaling, so typically we standardize (e.g. Z-score) features before fitting model (Sklearn `StandardScaler`)

Scikit-Learn : L2 Regularized Regression

`sklearn.linear_model`.Ridge

class sklearn.linear_model.Ridge(*alpha=1.0*, ***, *fit_intercept=True*, *normalize='deprecated'*, *copy_X=True*, *max_iter=None*, *tol=0.001*, *solver='auto'*, *positive=False*, *random_state=None*) ¶ [source]

alpha : *{float, ndarray of shape (n_targets,)}, default=1.0*

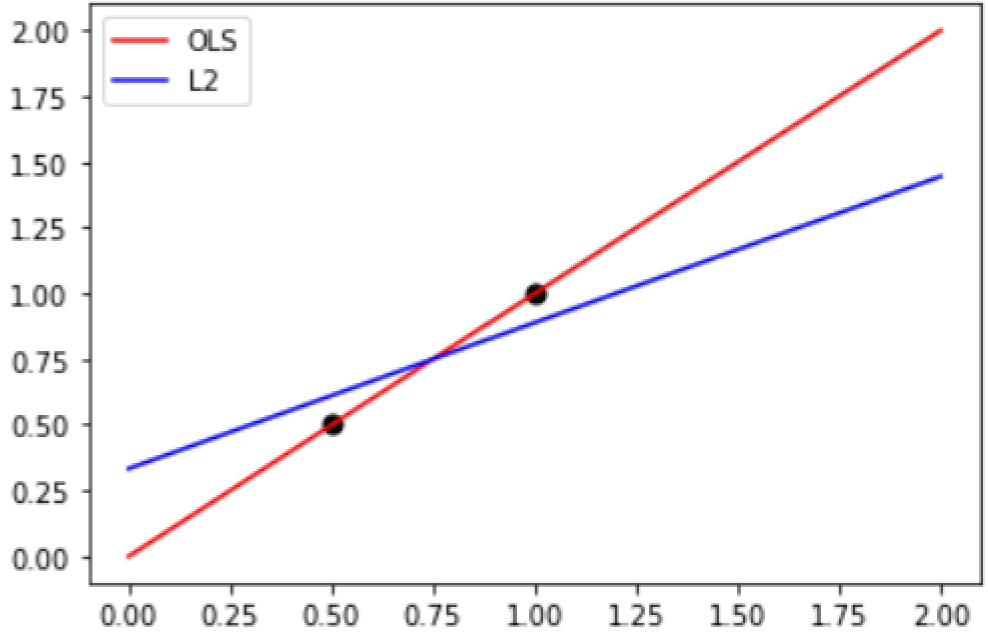
Regularization strength; must be a positive float. Regularization improves the conditioning of the problem and reduces the variance of the estimates. Larger values specify stronger regularization. Alpha corresponds to `1 / (2C)` in other linear models such as `LogisticRegression` or `LinearSVC`. If an array is passed, penalties are assumed to be specific to the targets. Hence they must correspond in number.

Alpha is what we have been calling λ

Scikit-Learn : L2 Regularized Regression

Define and fit OLS and L2 regression,

```
ols=linear_model.LinearRegression()
ols.fit(X_train, y_train)
ridge=linear_model.Ridge(alpha=0.1)
ridge.fit(X_train, y_train)
```



Plot results,

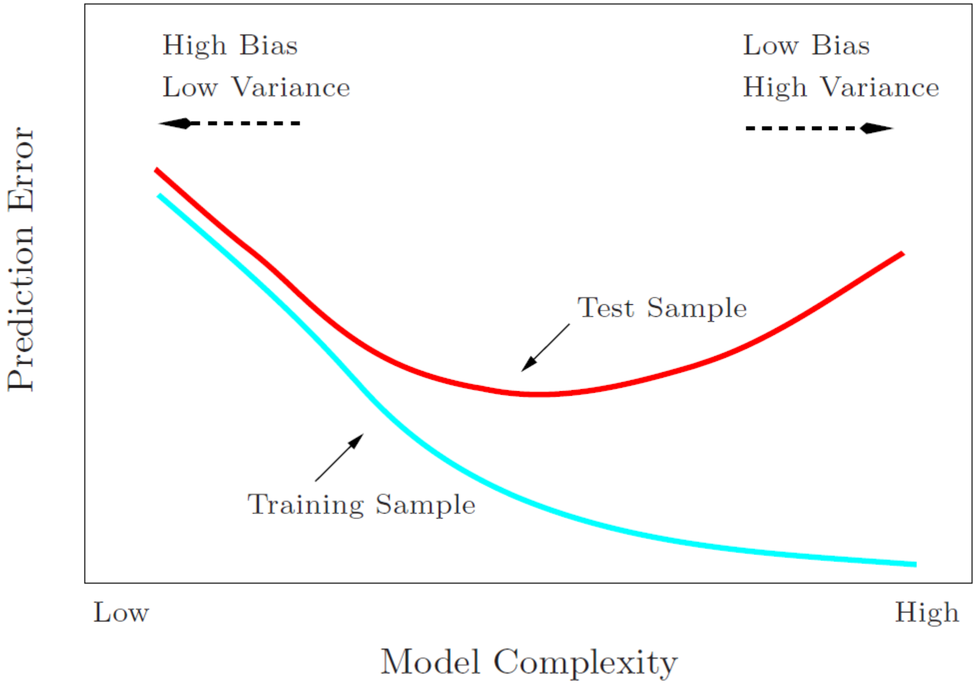
```
fig, ax = plt.subplots()
ax.scatter(X_train, y_train, s=50, c="black", marker="o")
ax.plot(X_test, ols.predict(X_test), color="red", label="OLS")
ax.plot(X_test, ridge.predict(X_test), color="blue", label="L2")

plt.legend()
plt.show()
```

L2 (Ridge) reduces impact of any single data point

Choosing Regularization Strength

We need to tune regularization strength to avoid over/under fitting…

$$w^{\mathrm{L2}} = \arg\min_{w} \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \frac{\lambda}{2} \|w\|^2$$



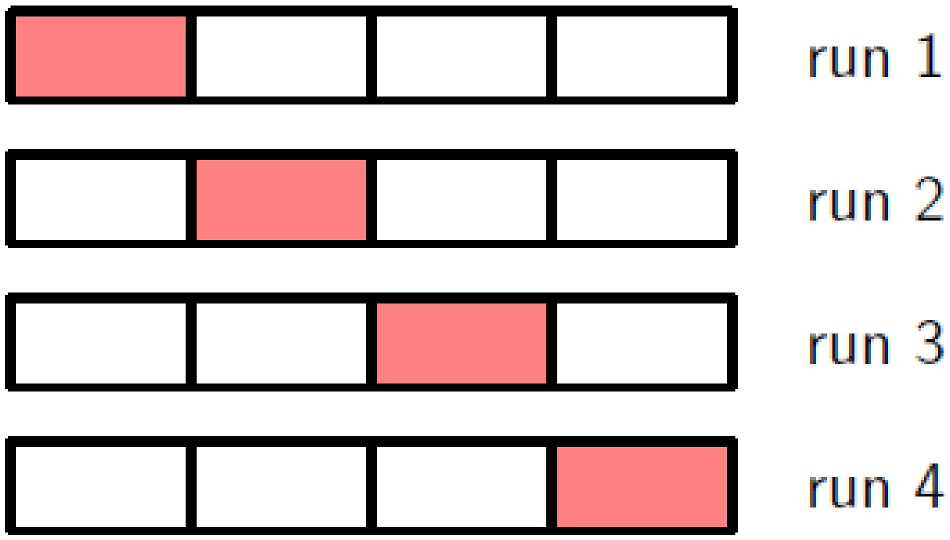
Recall bias/variance tradeoff

Error = Bias^2 + Variance

High regularization *reduces* model complexity: *increases* bias / *decreases* variance

How should we properly tune λ?

Cross-Validation



N-fold Cross Validation Partition training data into N “chunks” and for each run select one chunk to be validation data

For each run, fit to training data (N-1 chunks) and measure accuracy on validation set. Average model error across all runs.

Drawback Need to perform training N times.

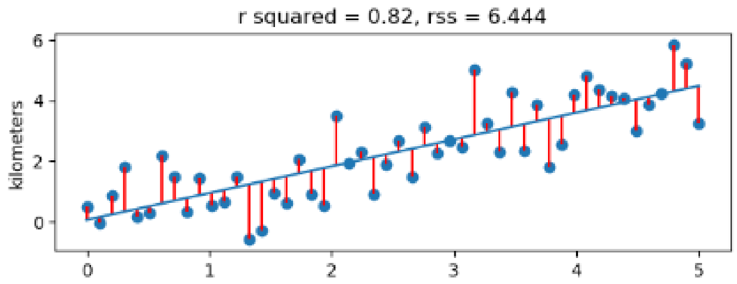
Source: Bishop, C. PRML

Model Selection for Linear Regression

A couple of common metrics for model selection…

Residual Sum-of-squared Errors The total squared residual error on the held-out validation set,

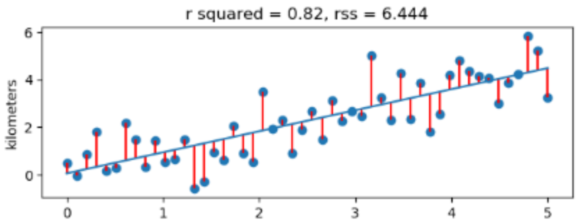
$$\text{RSS} = \sum_{i=1}^{N} (y_i - w^T x_i)^2$$



Coefficient of Determination Also called R-squared or R^2. Fraction of variation explained by the model.

Model selection metrics are known as "goodness of fit" measures

Coefficient of Determination R^2



Variance unexplained by Regression model

Residual Sum-of-Squares

$$R^2 = 1 - \frac{\text{RSS}}{\text{SS}} = 1 - \frac{\sum_{i=1}^{N}(y_i - w^T x_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}$$

Total variance in dataset

Variance using avg. prediction

Where: $\bar{y} = \frac{1}{N}\sum_i y_i$ is the average output

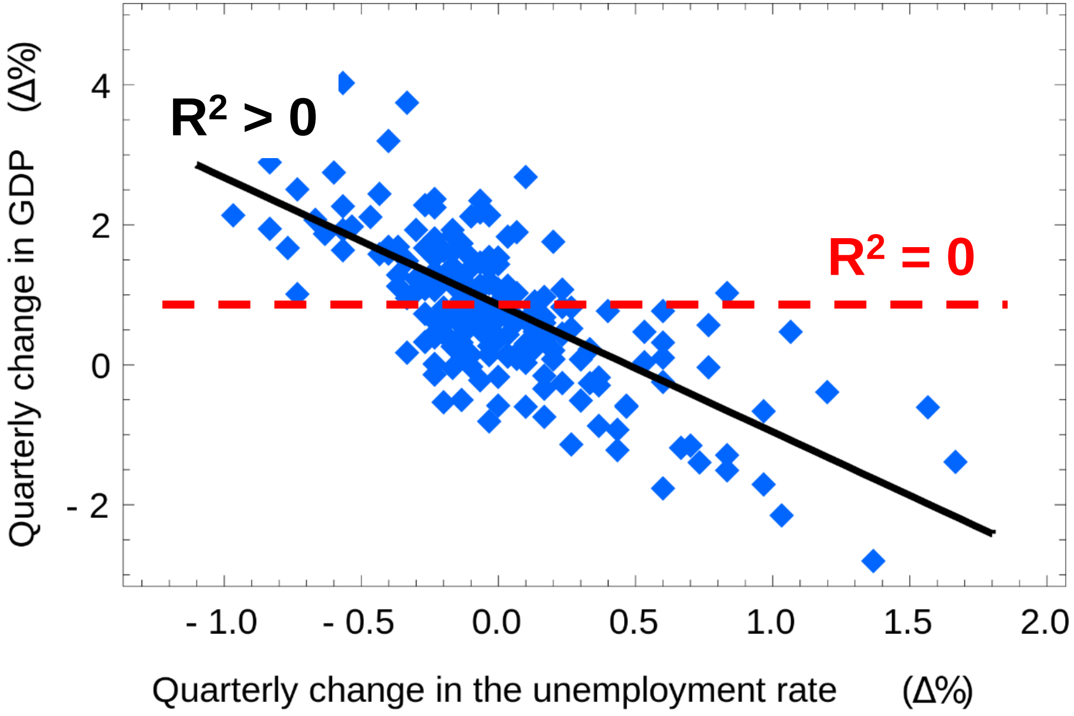
Coefficient of Determination R^2

$$R^2 = 1 - \frac{\text{RSS}}{\text{SS}} = 1 - \frac{\sum_{i=1}^{N}(y_i - w^T x_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}$$

Maximum value R^2=1.0 means model explains *all variation* in the data

Maximum value R^2=0 means model is as good as predicting average response

R^2<0 means model is worse than predicting average output



"Shrinkage" Feature Selection

Down-weight features that are not useful for prediction…

Quadratic penalty $\lambda \|w\|^2$ down-weights (shrinks) features that are not useful for prediction

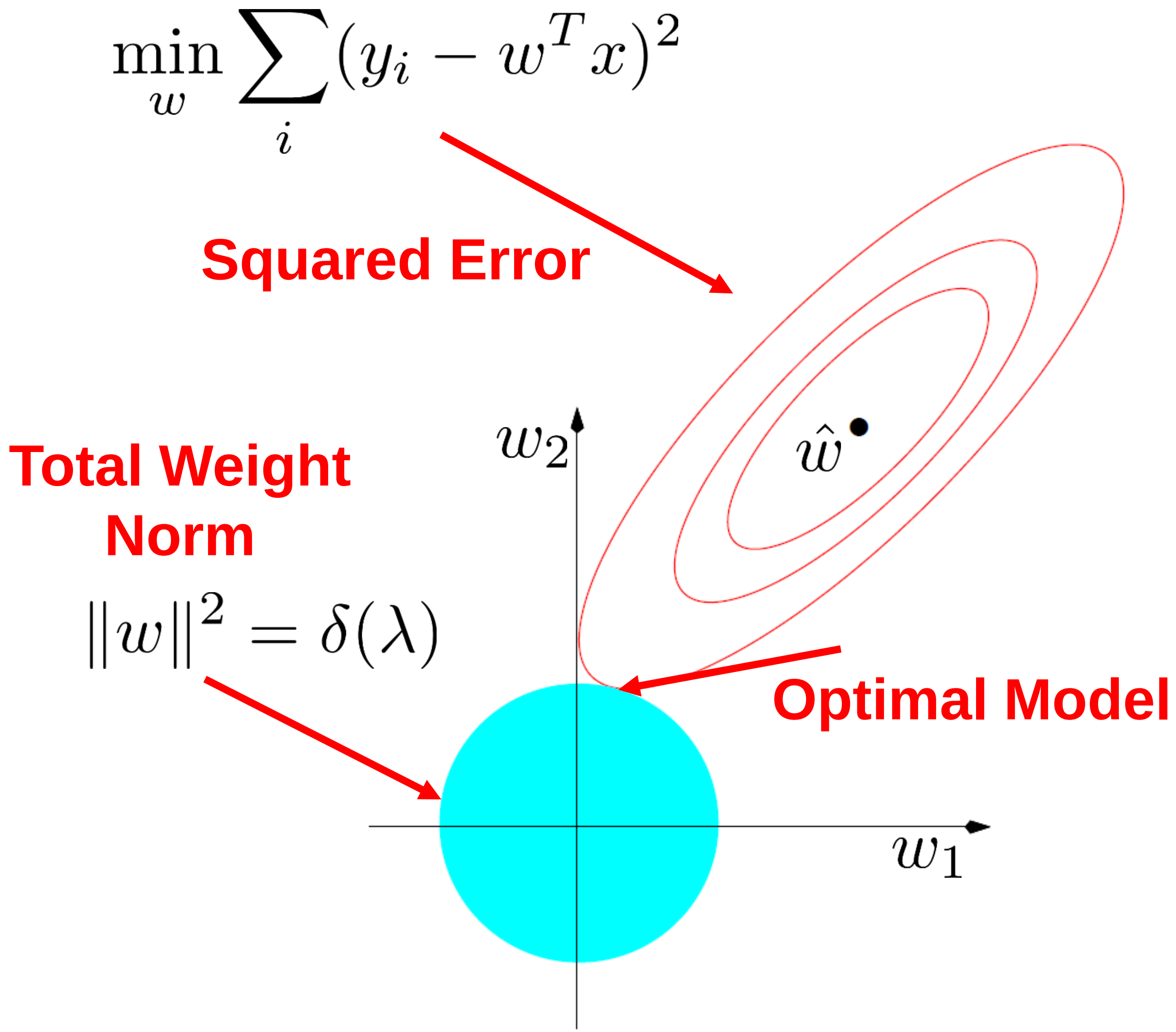
Term	LS	Ridge
Intercept	2.465	2.452
lcavol	0.680	0.420
lweight	0.263	0.238
age	−0.141	−0.046
lbph	0.210	0.162
svi	0.305	0.227
lcp	−0.288	0.000
gleason	−0.021	0.040
pgg45	0.267	0.133

Example *Prostate Cancer Dataset* measures prostate-specific cancer antigen with features: age, log-prostate weight (lweight), log-benign prostate hyperplasia (lbph), Gleason score (gleason), seminal vesical invasion (svi), etc.

L2 regularization learns zero-weight for log capsular penetration (lcp)

[Source: Hastie et al. (2001)]

Regularized regression: Constrained Optimization Perspective



- **<u>Fact:</u>** the solution of

$$\arg\min_{w} \|Xw - y\|_2^2 + \lambda \|w\|_2 ,$$

Is equivalent to the solution of the constrained optimization problem:

$$\arg\min_{w: \|w\|_2 \leq \delta(\lambda)} \|Xw - y\|_2^2$$

for some $\delta(\lambda)$

L2 penalized regression rarely learns feature weight that are *exactly zero…*

[Source: Hastie et al. (2001)]

Regularized Least Squares

Ordinary least-squares estimation (no regularizer),

$$w^{\mathrm{OLS}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2$$

L2-regularized Least-Squares (Ridge)

Quadratic Penalty

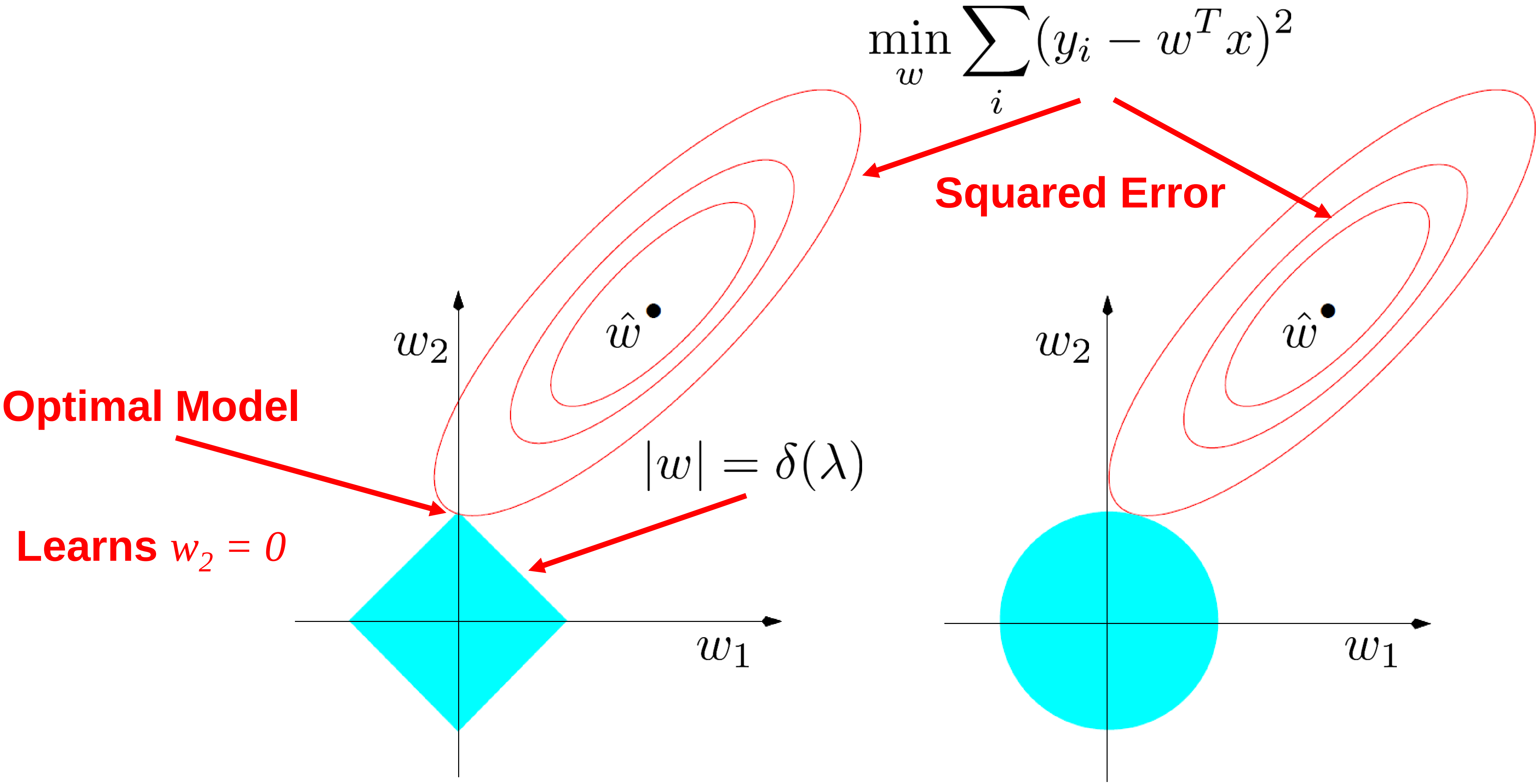
$$w^{\mathrm{L2}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \frac{\lambda}{2}\|w\|^2$$

L1-regularized Least-Squares (LASSO)

Absolute Value (L1) Penalty

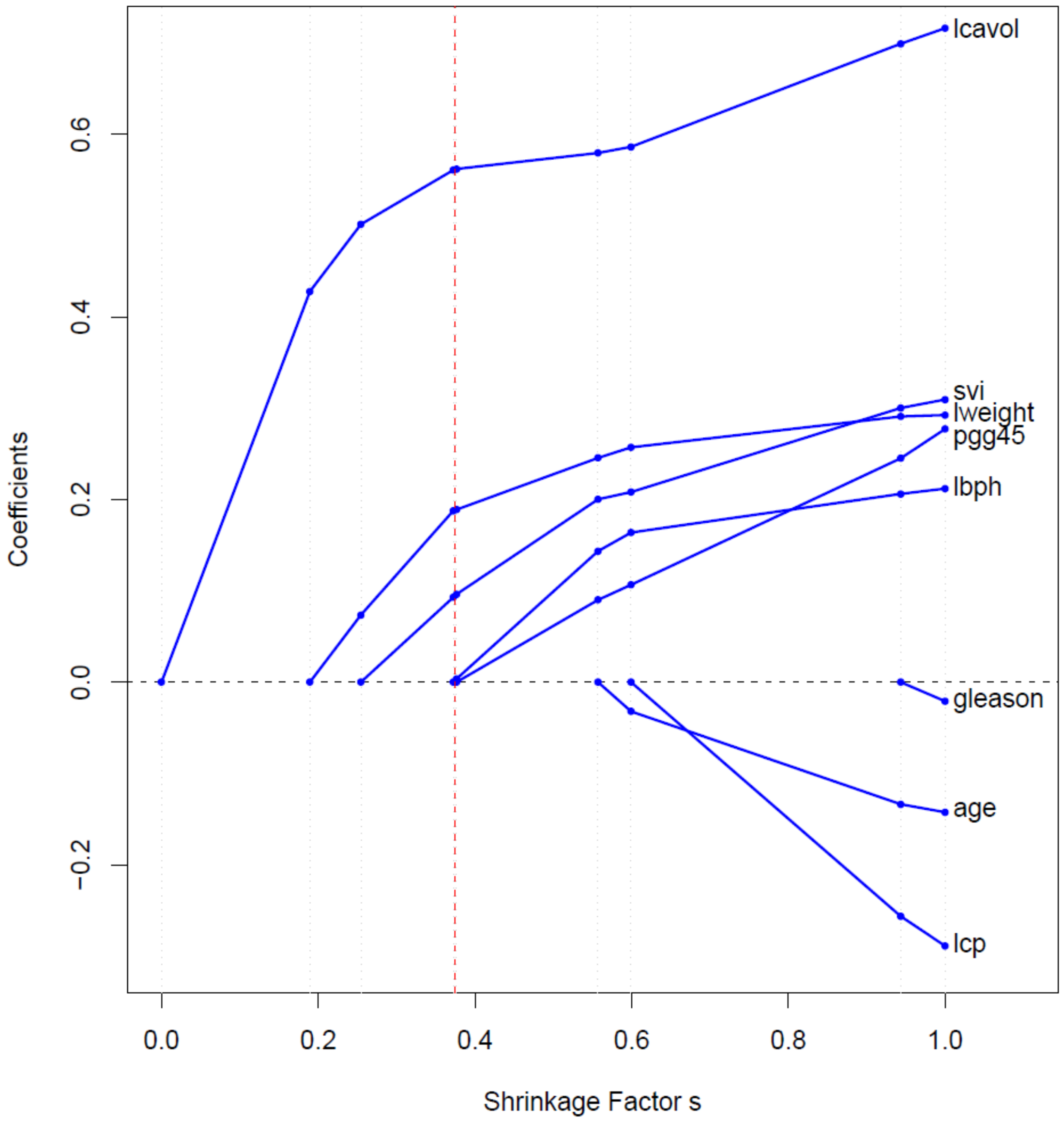
$$w^{\mathrm{L1}} = \arg\min_w \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \lambda|w|$$

L1 Regularized Least-Squares



Able to zero-out weights that are not predictive…

Feature Weight Profiles

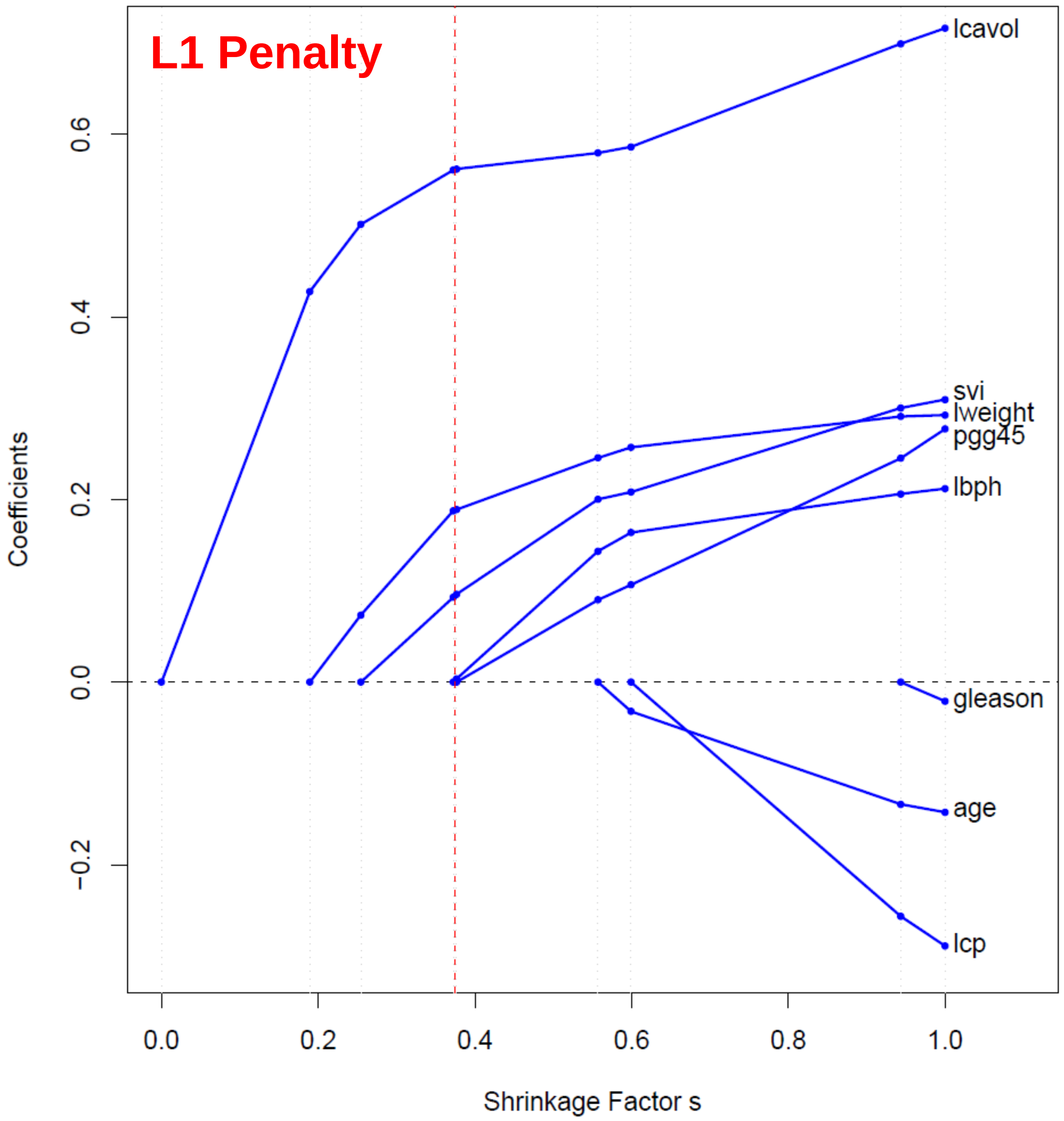


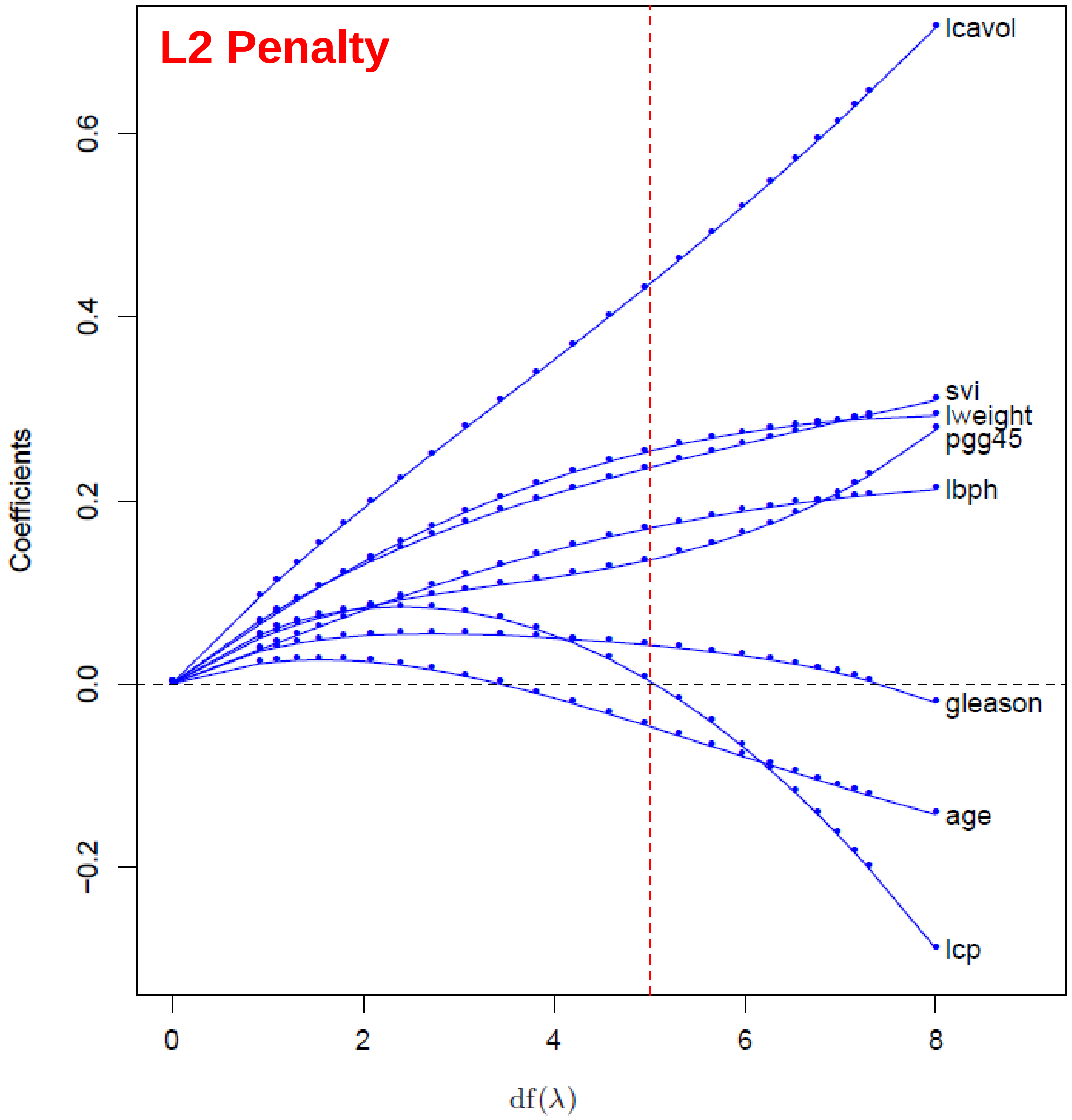
Varying regularization parameter moderates *shrinkage factor*

For moderate regularization strength weights for many features go to zero

- Induces *model sparsity*
- Ideal for high-dimensional settings
- Gracefully handles p>N case, for p features and N training data

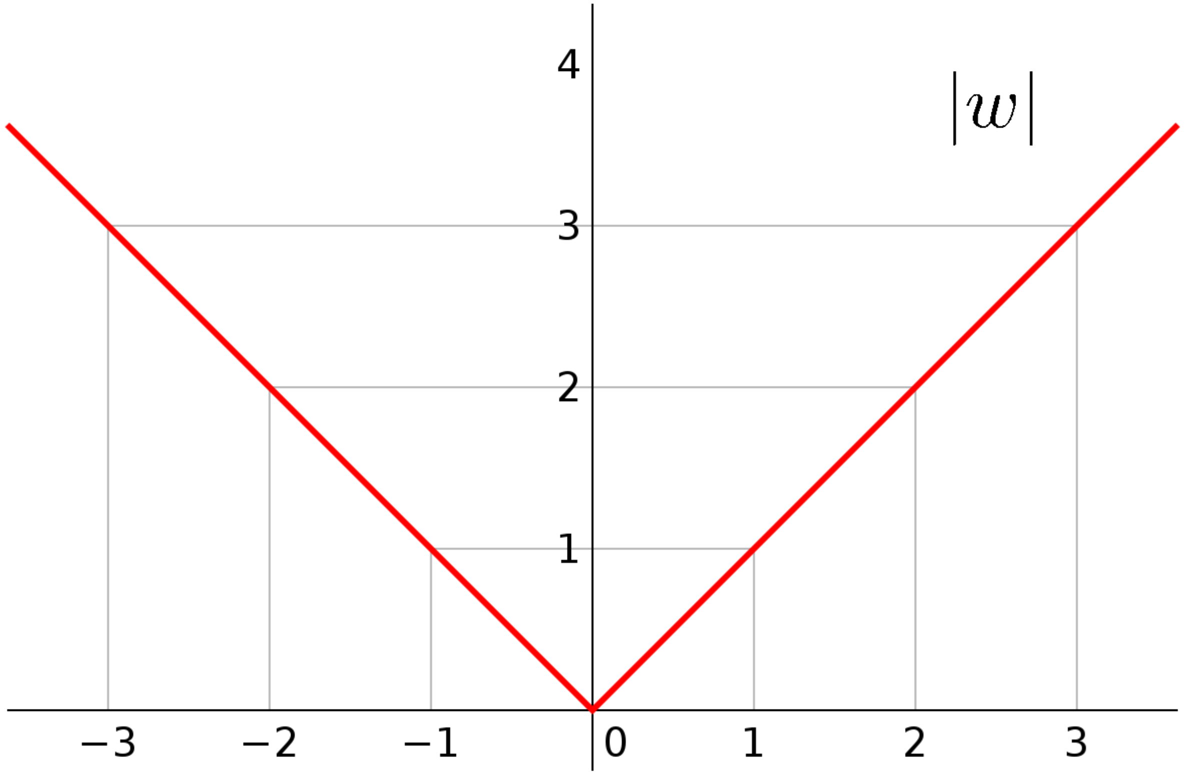
Feature Weight Profiles





Learning L1 Regularized Least-Squares

$$w^{\mathrm{L1}} = \arg\min_{\theta} \sum_{i=1}^{N} (y_i - w^T x_i)^2 + \lambda |w|$$



Not differentiable…

$$\frac{d}{dx}|x|$$

…doesn’t exist at x=0

Can’t set derivatives to zero as in the L2 case!

Learning L1 Regularized Least-Squares

- Not differentiable, no closed-form solution
- But it is convex! Can be solved by standard convex optimization packages (e.g. CVXPY)
- Efficient optimization algorithms exist
- *Least Angle Regression* (LAR) computes **full solution path** for a range of values λ
- Can be solved as efficiently as L2 regression

sklearn.linear_model.Lasso

class sklearn.linear_model.Lasso(*alpha=1.0*, ***, *fit_intercept=True*, *normalize='deprecated'*, *precompute=False*, *copy_X=True*, *max_iter=1000*, *tol=0.0001*, *warm_start=False*, *positive=False*, *random_state=None*, *selection='cyclic'*) ¶ [source]

Parameters:

alpha : *float, default=1.0*

Constant that multiplies the L1 term. Defaults to 1.0. `alpha = 0` is equivalent to an ordinary least square, solved by the `LinearRegression` object. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised. Given this, you should use the `LinearRegression` object.

fit_intercept : *bool, default=True*

Whether to calculate the intercept for this model. If set to False, no intercept will be used in calculations (i.e. data is expected to be centered).

precompute : *'auto', bool or array-like of shape (n_features, n_features), precompute*

Whether to use a precomputed Gram matrix to speed up calculations. The Gram matrix can also be passed as argument. For sparse input this option is always `False` to preserve sparsity.

copy_X : *bool, default=True*

If `True`, X will be copied; else, it may be overwritten.

Specialized methods for cross-validation…

sklearn.linear_model.LassoCV

class sklearn.linear_model.LassoCV(*, *eps=0.001*, *n_alphas=100*, *alphas=None*, *fit_intercept=True*, *normalize='deprecated'*, *precompute='auto'*, *max_iter=1000*, *tol=0.0001*, *copy_X=True*, *cv=None*, *verbose=False*, *n_jobs=None*, *positive=False*, *random_state=None*, *selection='cyclic'*) [source]

Computes solution using coordinate descent

sklearn.linear_model.LassoLarsCV

class sklearn.linear_model.LassoLarsCV(*, *fit_intercept=True*, *verbose=False*, *max_iter=500*, *normalize='deprecated'*, *precompute='auto'*, *cv=None*, *max_n_alphas=1000*, *n_jobs=None*, *eps=2.220446049250313e-16*, *copy_X=True*, *positive=False*) ¶ [source]

Uses *least angle regression* (LARS) to compute solution path

L1 Regression Cross-Validation

Perform L1 Least Squares (LASSO) 20-fold cross-validation,

```
model = LassoCV(cv=20).fit(X, y)
```

or

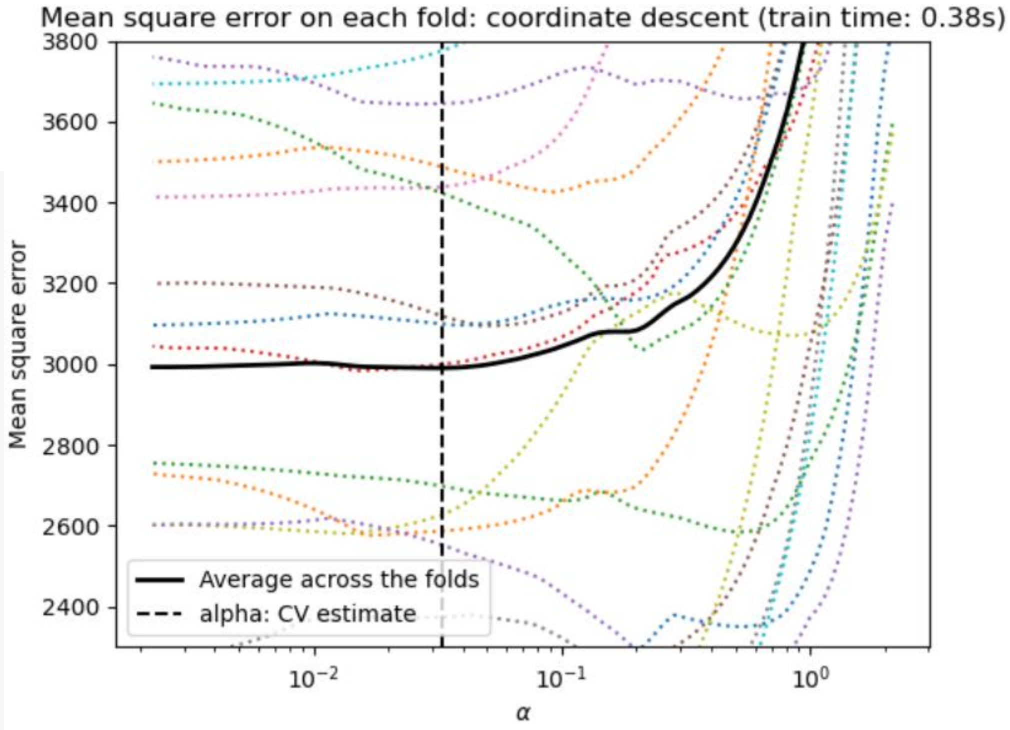
```
model = LassoLarsCV(cv=20, normalize=False).fit(X, y)
```

Plot solution path for range of alphas,

```
plt.figure()
ymin, ymax = 2300, 3800
plt.semilogx(model.alphas_ + EPSILON, model.mse_path_, ":")
plt.plot(
    model.alphas_ + EPSILON,
    model.mse_path_.mean(axis=-1),
    "k",
    label="Average across the folds",
    linewidth=2,
)
plt.axvline(
    model.alpha_ + EPSILON, linestyle="--", color="k", label="alpha: CV estimate"
)
```

All alphas_

Learned alpha_ (no “s”… annoying…)



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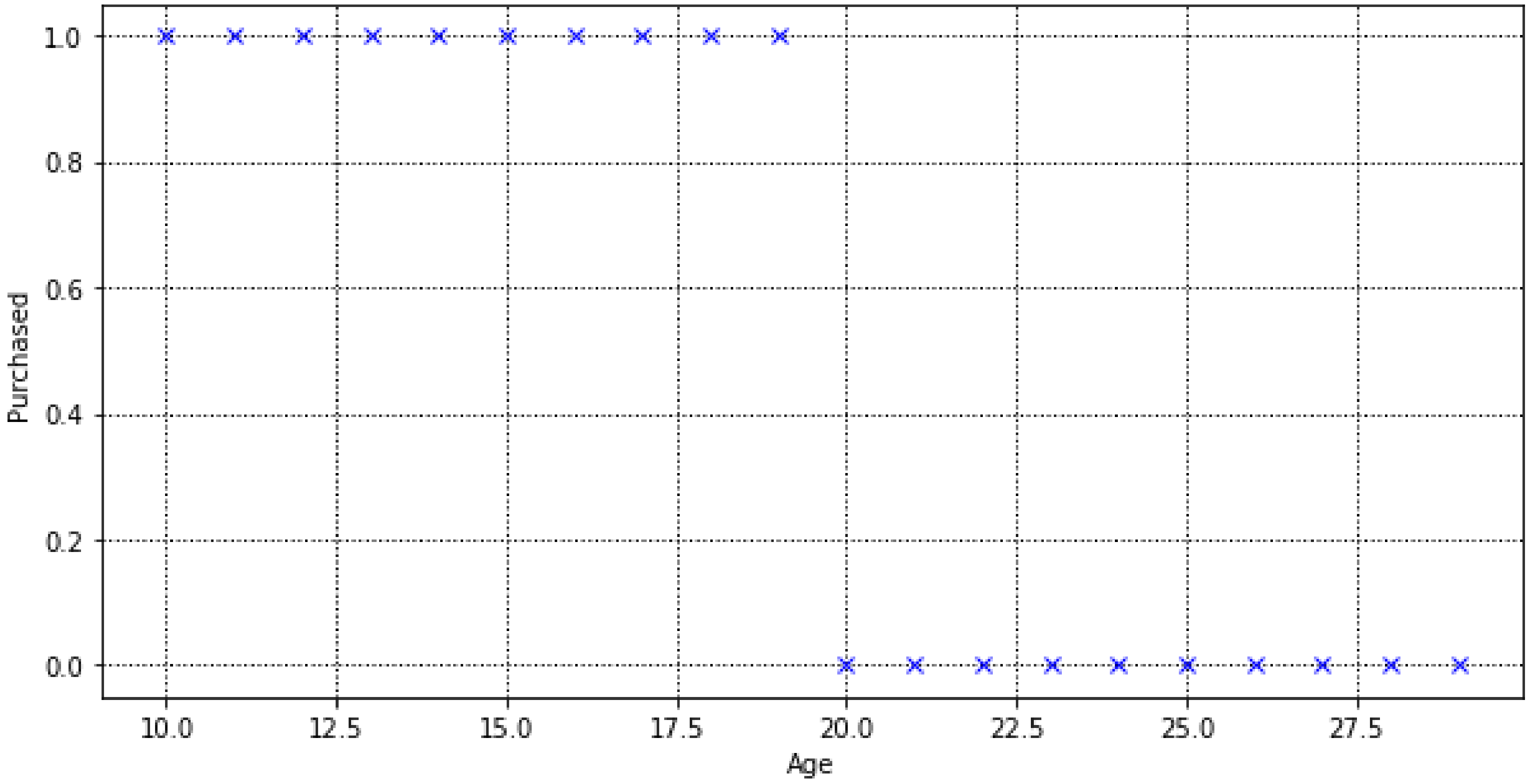
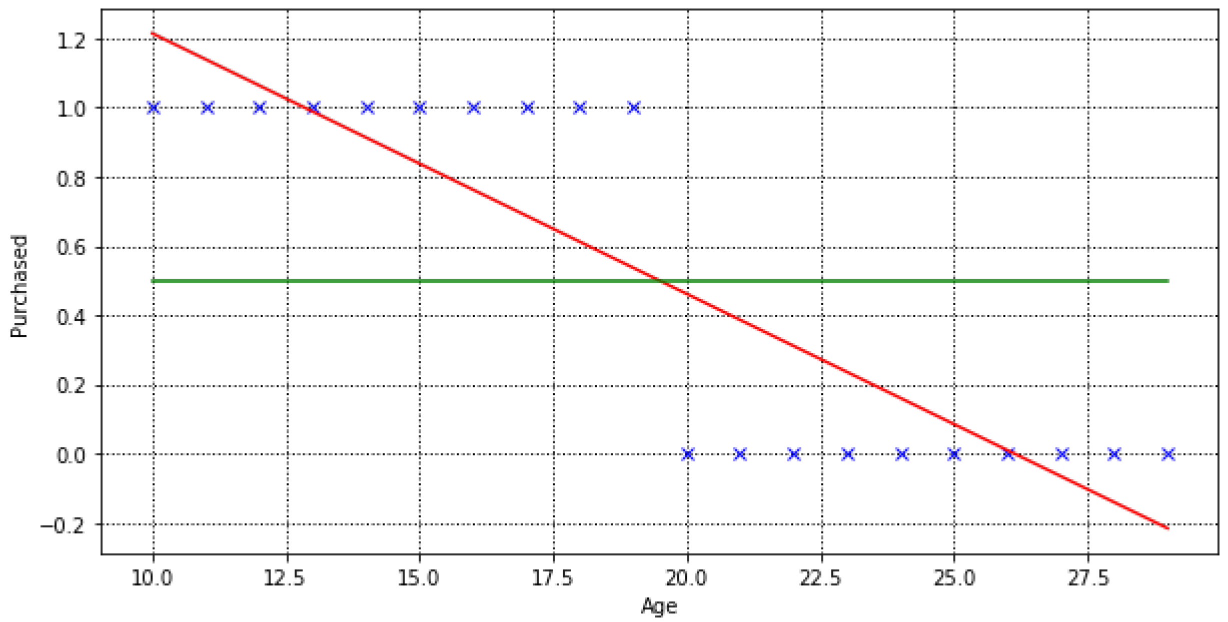
Classification as Regression

Suppose our response variables are binary y={0,1}. How can we use linear regression ideas to solve this classification problem?



https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Least squares classification: classification as regression



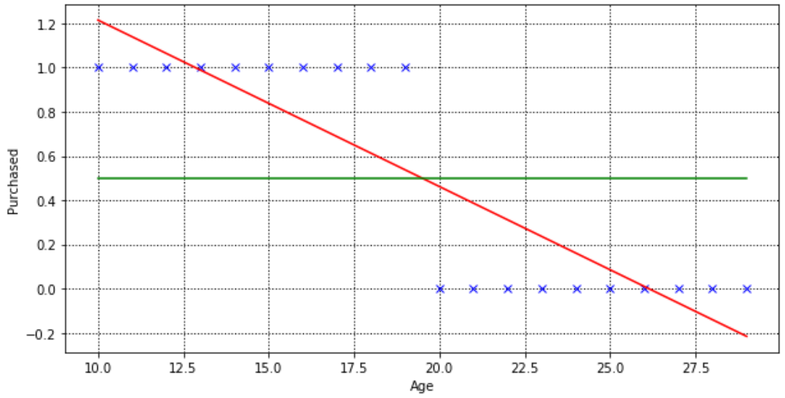
Idea Fit a least-square linear regressor *w* to the data (red). Classify points based on whether they are *above* or *below* the midpoint (green).

$$h(x) = I(w^T x \geq 0.5)$$

- This is a *discriminant* function, since it discriminates between classes
- It is a linear function and so is a *linear discriminant*
- We can call this approach **least squares classification**

https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Least squares classification: rationale



Recall: Bayes optimal classifier

$$h^*(x) = I\left(P(y = 1 \mid x) \geq 0.5\right)$$

(Why?)

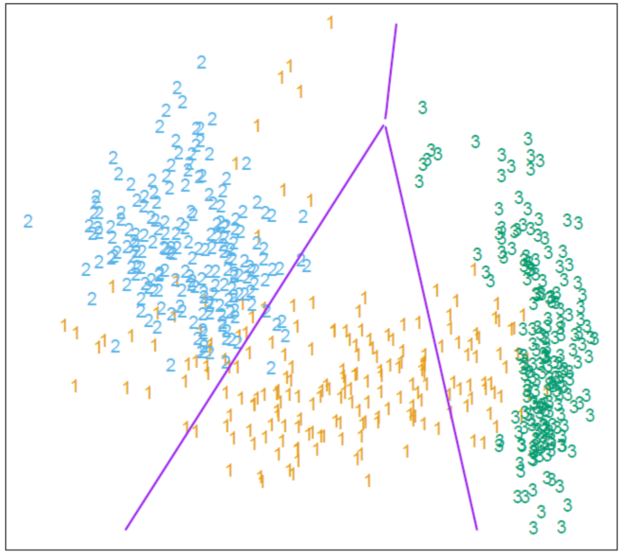
Recall the linear regression model, $p(y \mid x) = \mathcal{N}(w^T x, \sigma^2)$

So linear regression aims at predicting the expected value of y given x,

$$w^T x \approx \mathbf{E}[y \mid x] = P(y = 1 \mid x)$$

Thus $h(x) = I(w^T x \geq 0.5)$ should closely approximate the Bayes optimal classifier

Least squares classification: multiclass setting



Suppose we have K classes. Each example's label is represented by an *indicator vector*,

$$Y = (Y_1, \ldots, Y_K)$$

With $Y_k = 1$ if example is of class k,
e.g. for K=5, class 3, Y=(0,0,1,0,0).

For N training inputs create NxK matrix of outputs $\mathbf{Y}$ and solve,

$$\mathbf{W} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

W is NxK matrix of K linear regression models
each column is for a different class

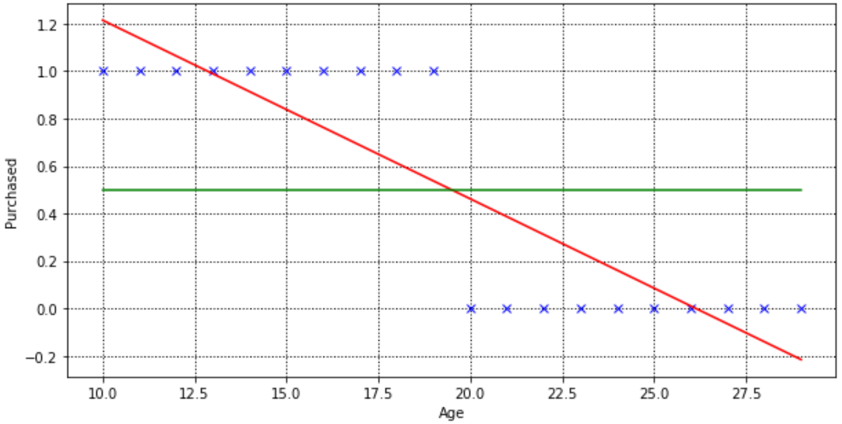
- Compute fitted output $f(x) = x^\top \mathbf{W}$ a K-vector
- Identify largest component and classify as,

$$C = \arg\max_k f_k(x)$$

This is an instance of multi-output linear regression

[Image: Hastie et al. (2001)]

Linear Probability Models



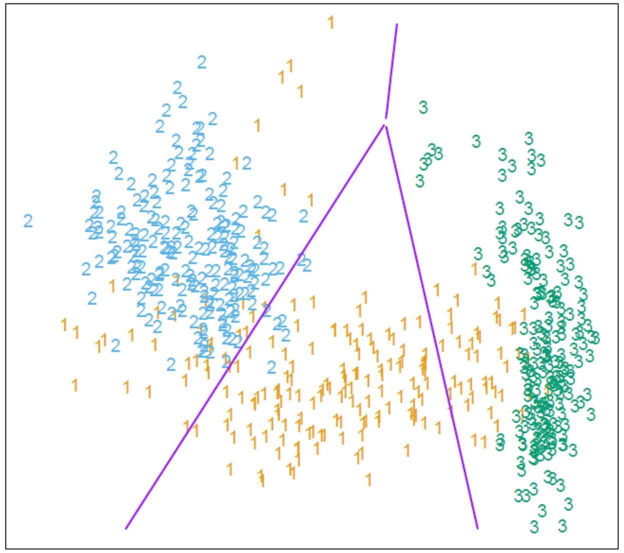
Binary Classification Linear model approximates probability of class assignment,

$$w^T x \approx p(y = 1|x)$$

Multiclass Classification Multiple decision boundaries, each approximated by the class-specific linear model,

$$\hat{f}_k(x) = W_{k:}^\top x$$

Where $W_{k:}$ is kth column of W



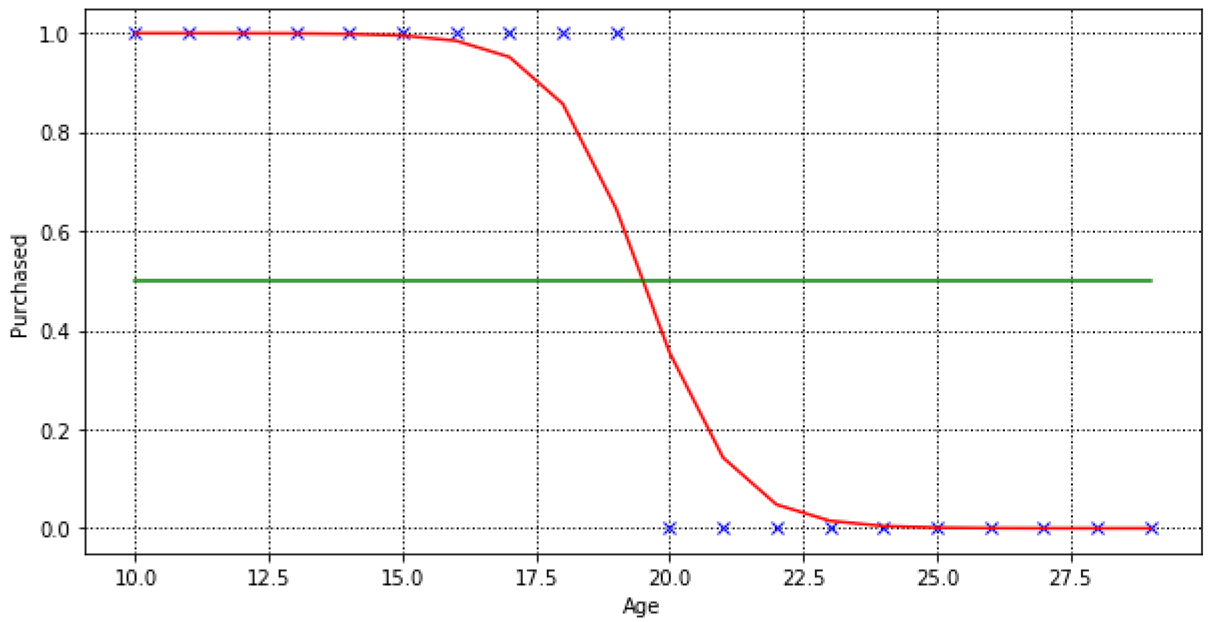
Approximates probability of class assignment,

$$\hat{f}_k(x) \approx p(y = k \mid x)$$

Any drawback with this approach?

Drawback: $w^T x$, $W_{k,:}^T x$ not guaranteed to be in [0,1]!

Logistic Regression

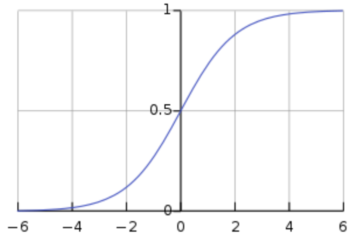


Idea Distort the prediction score in some way to map to [0,1] so that it is actually a probability.

$$f(x) = \sigma(w^T x)$$

Uses the *logistic* function,

$$\sigma(z) = \frac{\exp(z)}{1+\exp(z)}$$



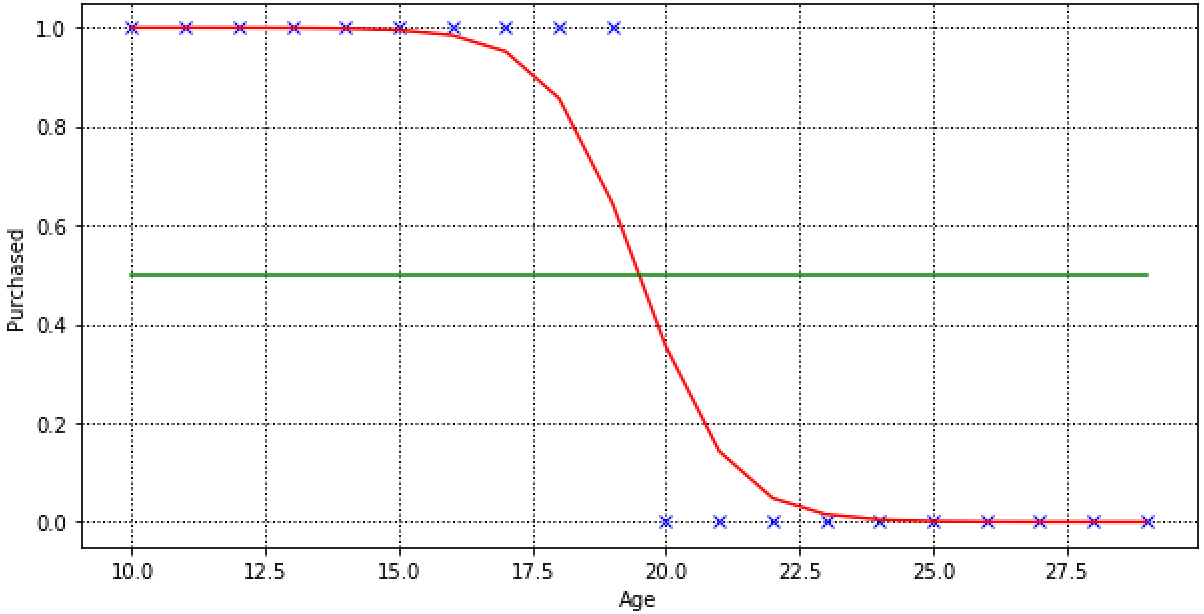
- Logistic function is a type of *sigmoid* or *squashing function*, since it maps any value to the range [0,1]

- Prediction now actually maps to a valid probability

$$f(x) = \sigma(w^T x) = p(y = 1 | w, x)$$

https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Logistic Regression: Decision Boundary



Bayes optimal prediction:

Predict 1 $\Leftrightarrow P(y = 1 \mid x) \geq 0.5$

$$\Leftrightarrow \text{(odd ratio)} \frac{P(y = 1 \mid x)}{P(y = 0 \mid x)} \geq 1$$

$$\Leftrightarrow \ln \frac{P(y = 1|x)}{P(y = 0|x)} \geq 0$$

Observe: logistic regression models: $p(y = 1|w, x) = \sigma(w^T x) = \frac{e^{w^T x}}{1+e^{w^T x}}$

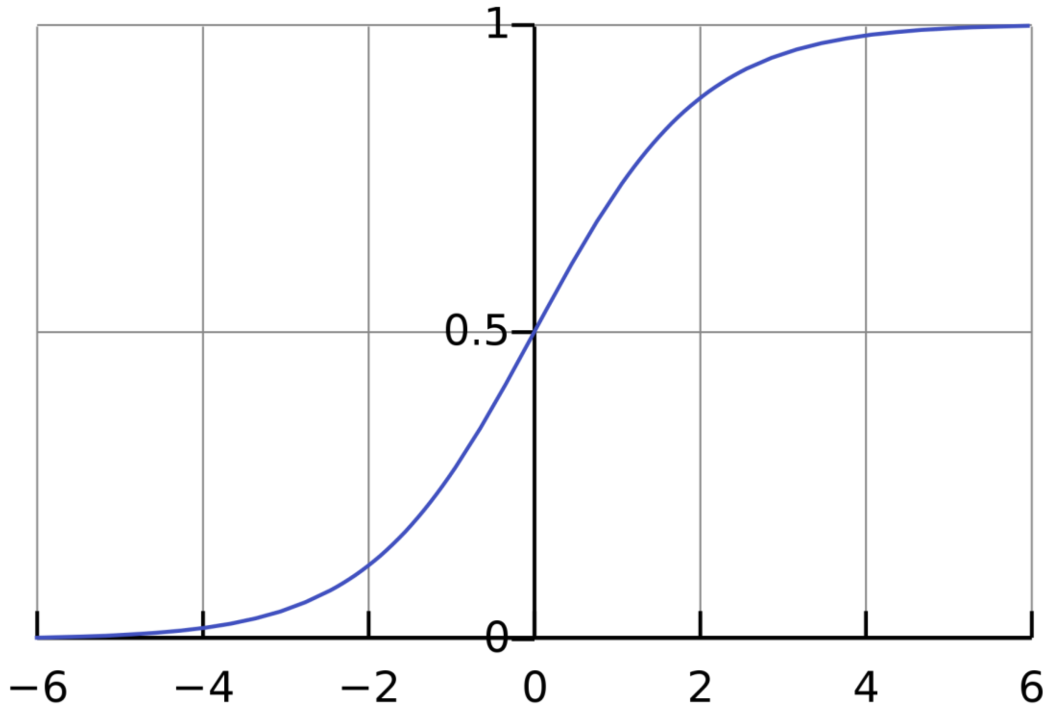
$$\implies \ln \frac{p(y = 1 \mid w, x)}{p(y = 0 \mid w, x)} = w^T x$$

This induces a *linear decision boundary*

Logistic regression gives a *linear classifier*

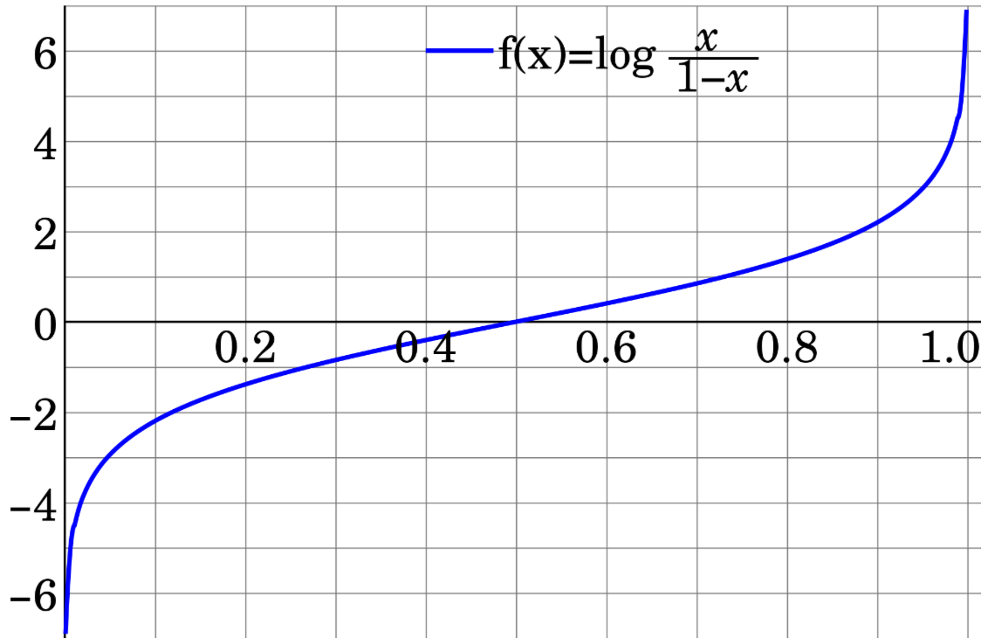
Logistic vs. Logit Transformations

Logistic Function



Maps $(-\infty, \infty)$ to [0,1]

Logit Function



Maps [0,1] to $(-\infty, \infty)$

Logistic also widely used in Neural Networks – for classification last layer is typically just a logistic regression

Logistic vs. Logit Transformations

Logistic function maps the linear prediction score to the interval [0,1],

$$\sigma(w^T x) = \frac{\exp(w^T x)}{1 + \exp(w^T x)}$$

Logit function is defined for probability values p in [0,1] as,

$$\text{logit}(p) = \log \frac{p}{1-p}$$

Logit is the *inverse* of the logistic function,

$$\text{logit}(\sigma(w^T x)) = w^T x$$

Logit is also the log-likelihood ratio, and thus induces decision boundary for our binary classifier

Multiclass Logistic Regression

Classification decision based on log-odd-ratio compared to final class,

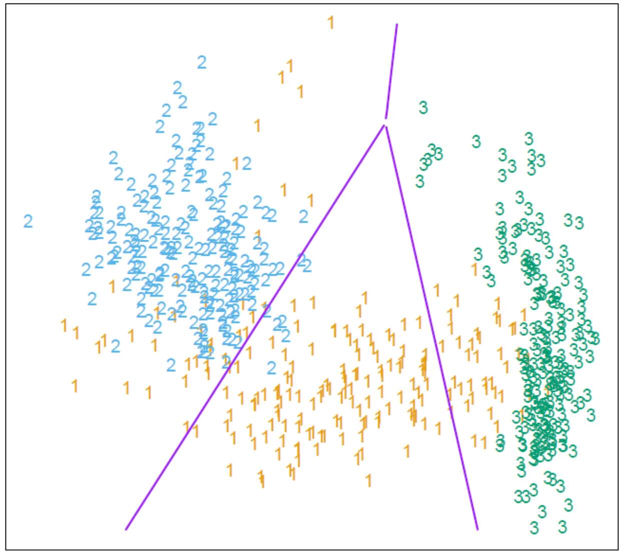
$p(C = i \mid x)$'s sum to 1

$$\log \frac{p(C=1 \mid x)}{p(C=K \mid x)} = w_1^T x$$

$$\log \frac{p(C=2 \mid x)}{p(C=K \mid x)} = w_2^T x$$

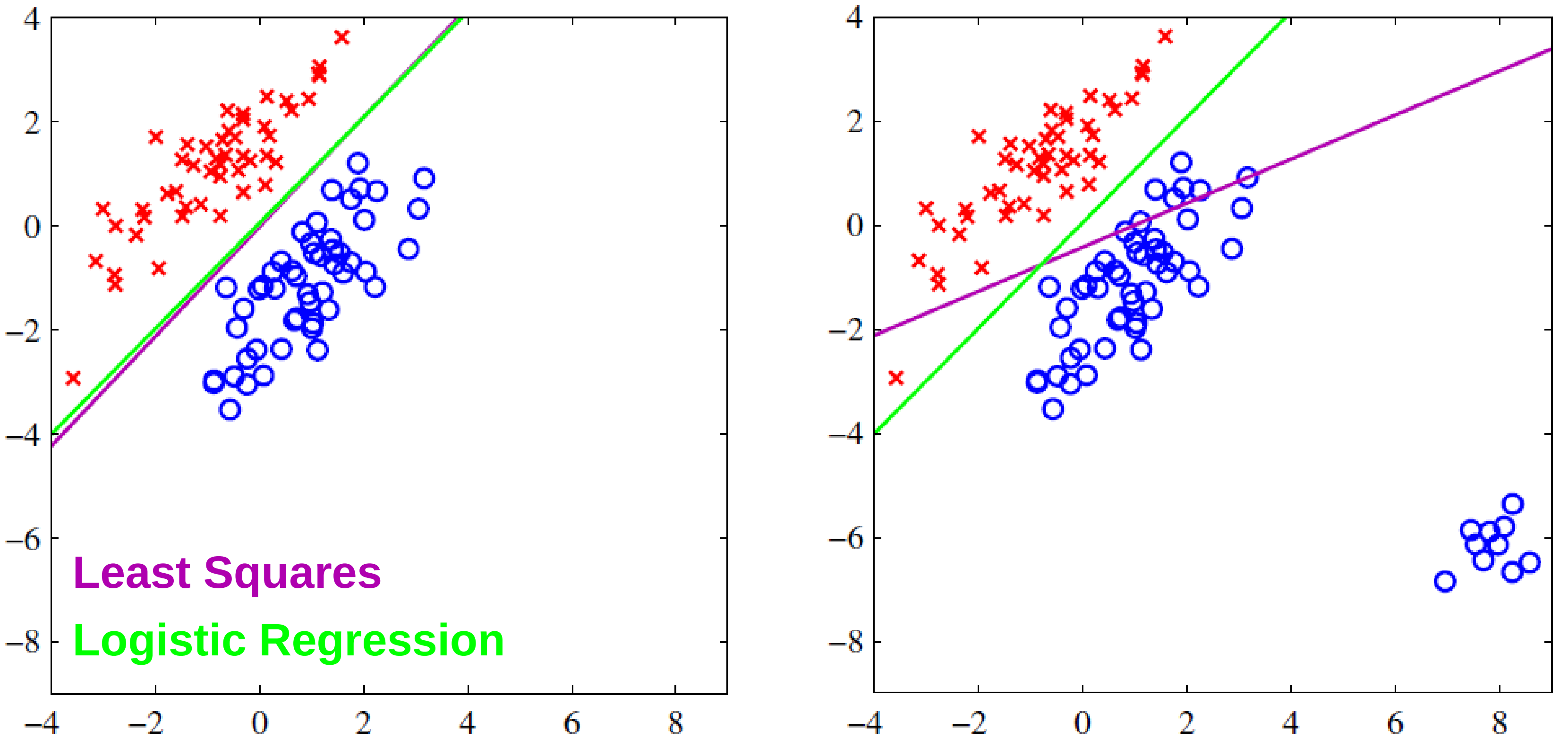
$$\vdots$$

$$\log \frac{p(C=K-1 \mid x)}{p(C=K \mid x)} = w_{K-1}^T x$$



Choice of denominator class is arbitrary, but use K by convention

Least Squares vs. Logistic Regression

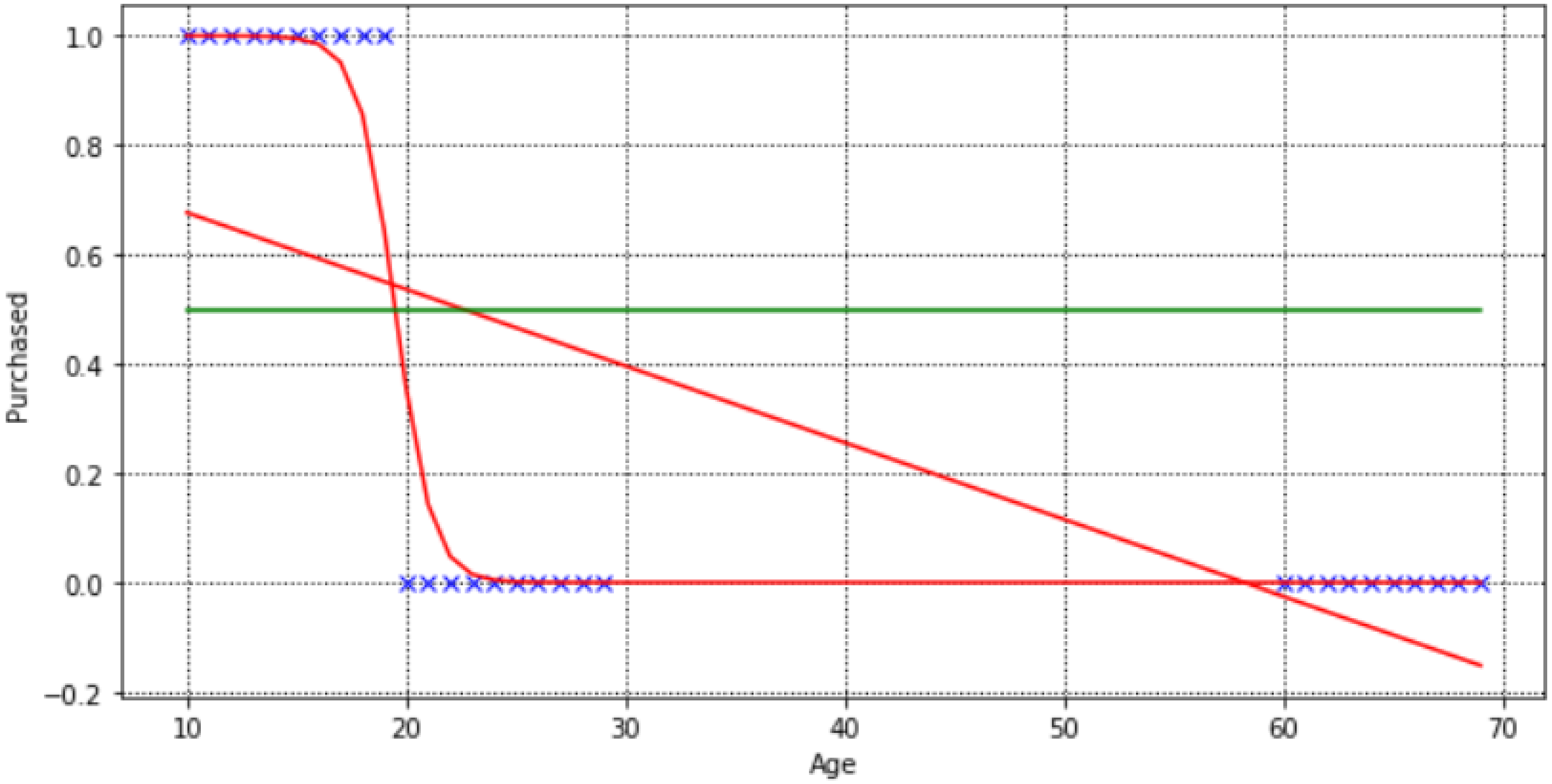


- Both models learn a linear decision boundary
- Least squares can be solved in closed-form (convex objective)
- Least squares is sensitive to outliers (need to do regularization)

[Source: Bishop "PRML"]

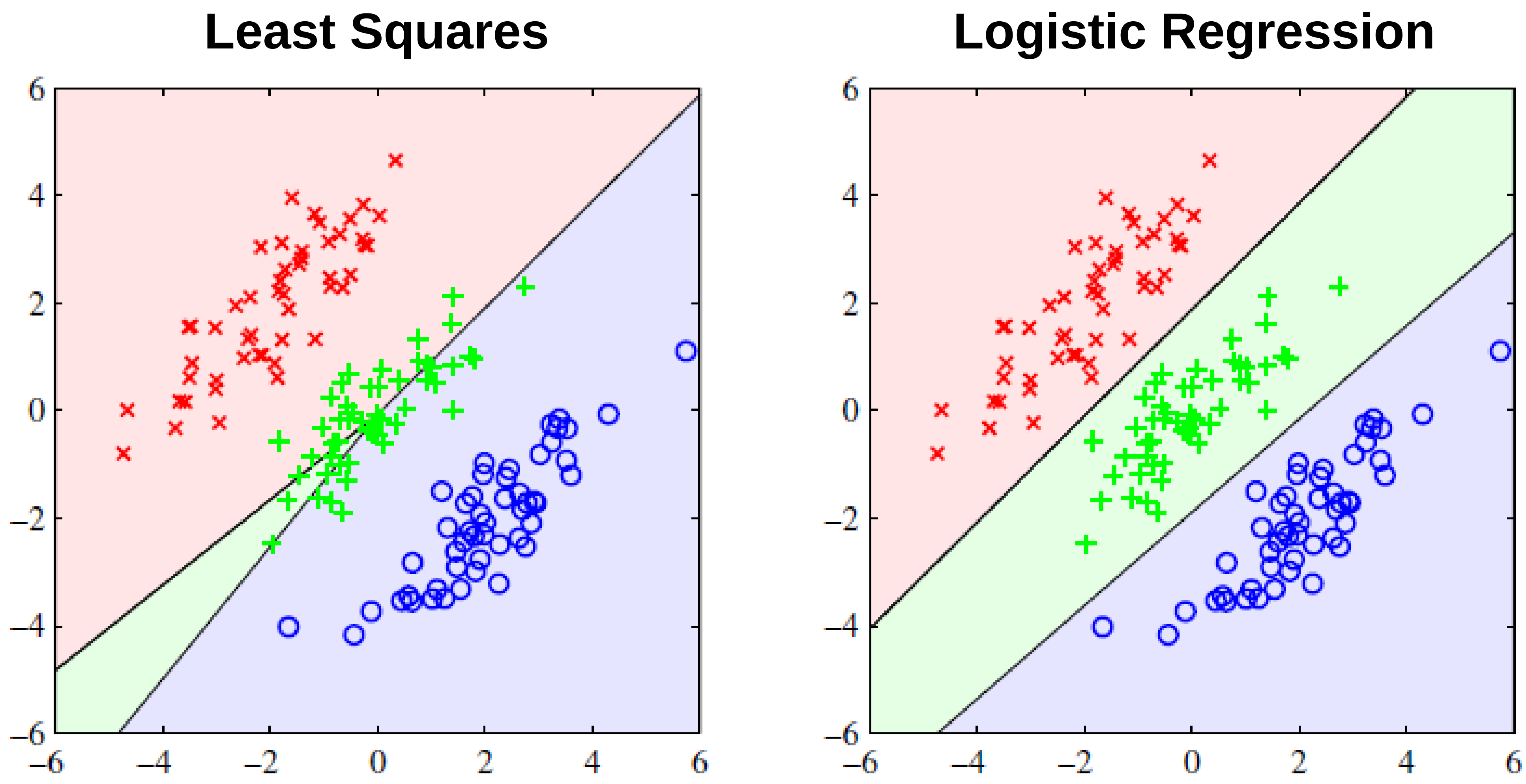
Least Squares vs. Logistic Regression

Similar qualitative comparisons in 1-dimension



https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Least Squares vs. Logistic Regression



[Source: Bishop "PRML"]

Logistic Regression: Model Training

Fit by maximum likelihood—start with the *binary* case

Recall: how is this defined?

Posterior probability of class assignment is Bernoulli,

$$p(y \mid x, w) = p(y = 1 \mid x, w)^y (1 - p(y = 1 \mid x, w))^{(1-y)}$$

Given N iid training data pairs the log-likelihood function is,

$$\begin{aligned}
\mathcal{L}_N(w) &= \sum_{i=1}^{N} \log p(y_i \mid x_i, w) \\
&= \sum_i \{y_i \log p(y_i = 1 \mid x_i, w) + (1 - y_i) \log p(y_i = 0 \mid x_i, w)\} \\
&= \sum_i \{y_i \log \sigma(w^T x_i) + (1 - y_i) \log(1 - \sigma(w^T x_i))\} \\
&= \sum_i \left\{y_i w^T x_i - \log\left(1 + e^{w^T x_i}\right)\right\}
\end{aligned}$$

Fitting Logistic Regression

$$w^{\mathrm{MLE}} = \arg\max_{w} \sum_{i} \left\{ y_i w^T x_i - \log\left(1 + e^{w^T x_i}\right) \right\}$$

This is a convex optimization problem => stationary points are optimal

Computing the derivatives with respect to each element w_d,

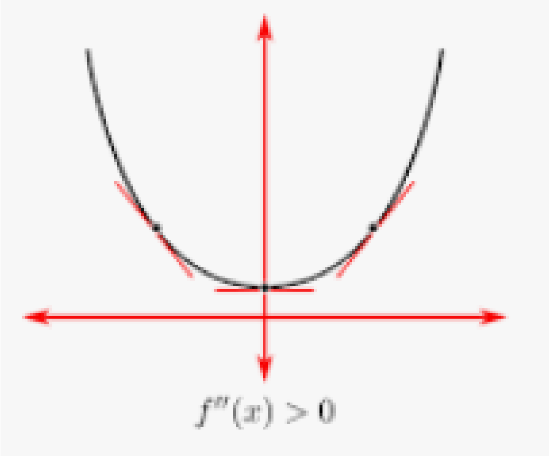
$$\frac{\partial \mathcal{L}}{\partial w_d} = \sum_{i} x_{di} \left(y_i - \frac{e^{w^T x_i}}{1 + e^{w^T x_i}} \right) = 0$$

- For D features this gives us D equations and D unknowns
- But equations are nonlinear and can't be solved
- Can use standard convex optimization toolbox (CVXPY) to solve it
- Can also be solved with Newton's method (Iterative Weighted Least Squares)

https://retostauffer.github.io/Rfoehnix/articles/logisticregression.html

Checking convexity – a toolkit

- How to check if function f is convex?
  - Idea 1: checking definition
    - for all $u, v, \alpha \in [0,1]$, $f(\alpha u + (1-\alpha)v) \leq \alpha f(u) + (1-\alpha)f(v)$
  - Idea 2: checking second order derivative
    - Fact: for univariate, 2nd order differentiable f, f is convex $\Leftrightarrow f''(u) \geq 0$ for all u



- E.g. $f(z) = \ln(1 + e^z)$
- How about multivariate f?

Checking convexity – a toolkit

- Fact: for multivariate, 2nd order differentiable f, f is convex $\Leftrightarrow$ its Hessian $\nabla^2 f(u) \succcurlyeq 0$ for all u
- $\succcurlyeq$: positive semidefinite (psd) partial order (Loewner order)
  - $A \succcurlyeq 0 \Leftrightarrow A$ is psd
- Exercise: verify that
$$F(w) = \sum_i \left\{ y_i w^T x_i - \log\left(1 + e^{w^T x_i}\right) \right\}$$
  is concave in w by checking its Hessian
- Is there an easier way?

Checking convexity – a toolkit

- Linear functions are both convex and concave
- Norms are convex
- If f, g be convex, then
  - max{f(x), g(x)} is convex
  - f(x) + g(x) is convex
  - if g is nondecreasing, then h(x) := g(f(x)) is convex => e.g., $h(w) = ||w||^2$
- f is concave, g is convex and nonincreasing, then h(x) := g(f(x)) is convex. e.g., $h(x) = \frac{1}{\log(1+x)}, x \geq 0$
- Convexity is invariant under affine maps: if f is convex, then $f(Ax + b)$ is also convex where $A \in \mathbb{R}^{n \times d}, b \in \mathbb{R}^n$

$$F(w) = \sum_i \left\{ y_i w^T x_i - \log\left(1 + e^{w^T x_i}\right) \right\}$$

sklearn.linear_model.LogisticRegression

class sklearn.linear_model.LogisticRegression(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) ¶ [source]

penalty : *{'l1', 'l2', 'elasticnet', 'none'}, default='l2'*

Specify the norm of the penalty:

- `'none'`: no penalty is added;
- `'l2'`: add a L2 penalty term and it is the default choice;
- `'l1'`: add a L1 penalty term;
- `'elasticnet'`: both L1 and L2 penalty terms are added.

Can also incorporate regularization in logistic regression

tol : *float, default=1e-4*

Tolerance for stopping criteria.

C : *float, default=1.0*

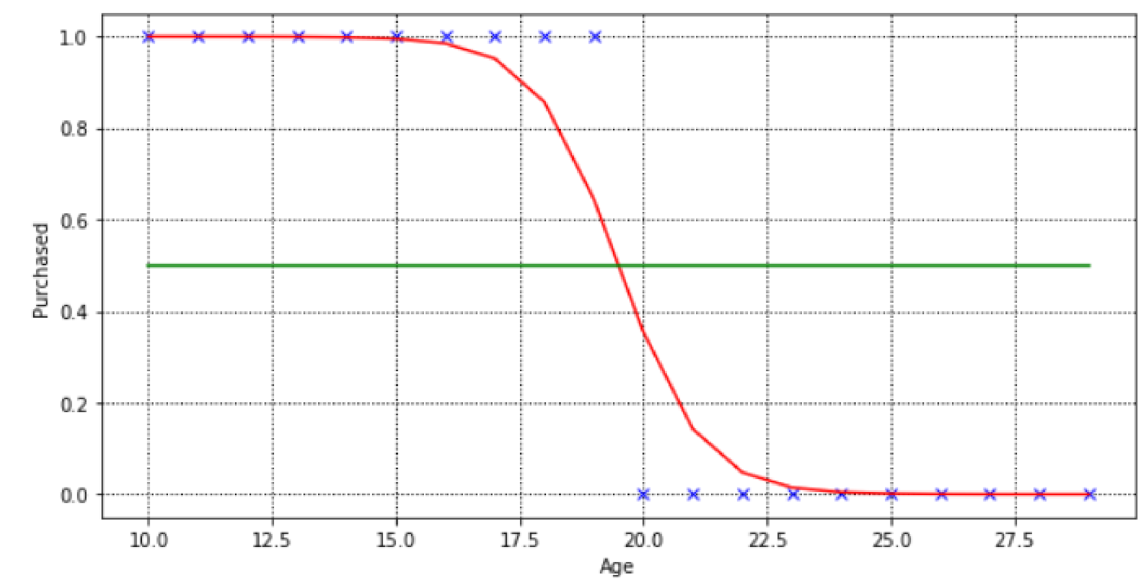
Inverse of regularization strength; must be a positive float. Like in support vector machines, smaller values specify stronger regularization.

Scikit-Learn Logistic Regression

```python
_ = log_regression.fit(pd.DataFrame(x), y)

y_pred = log_regression.predict_proba(pd.DataFrame(x))
log_y_pred_1 = [item[1] for item in y_pred]

fig = plt.figure(figsize=(10,5))
xlabel = 'Age'
ylabel = 'Purchased'
plt.xlabel(xlabel)
plt.ylabel(ylabel)
plt.grid(color='k', linestyle=':', linewidth=1)
plt.plot(x, y, 'xb')
plt.plot(x, log_y_pred_1, '-r')
_ = plt.plot(x, line_point_5,'-g')
```



Function `predict_proba(X)` returns prediction of class assignment probabilities (just a number in binary case)

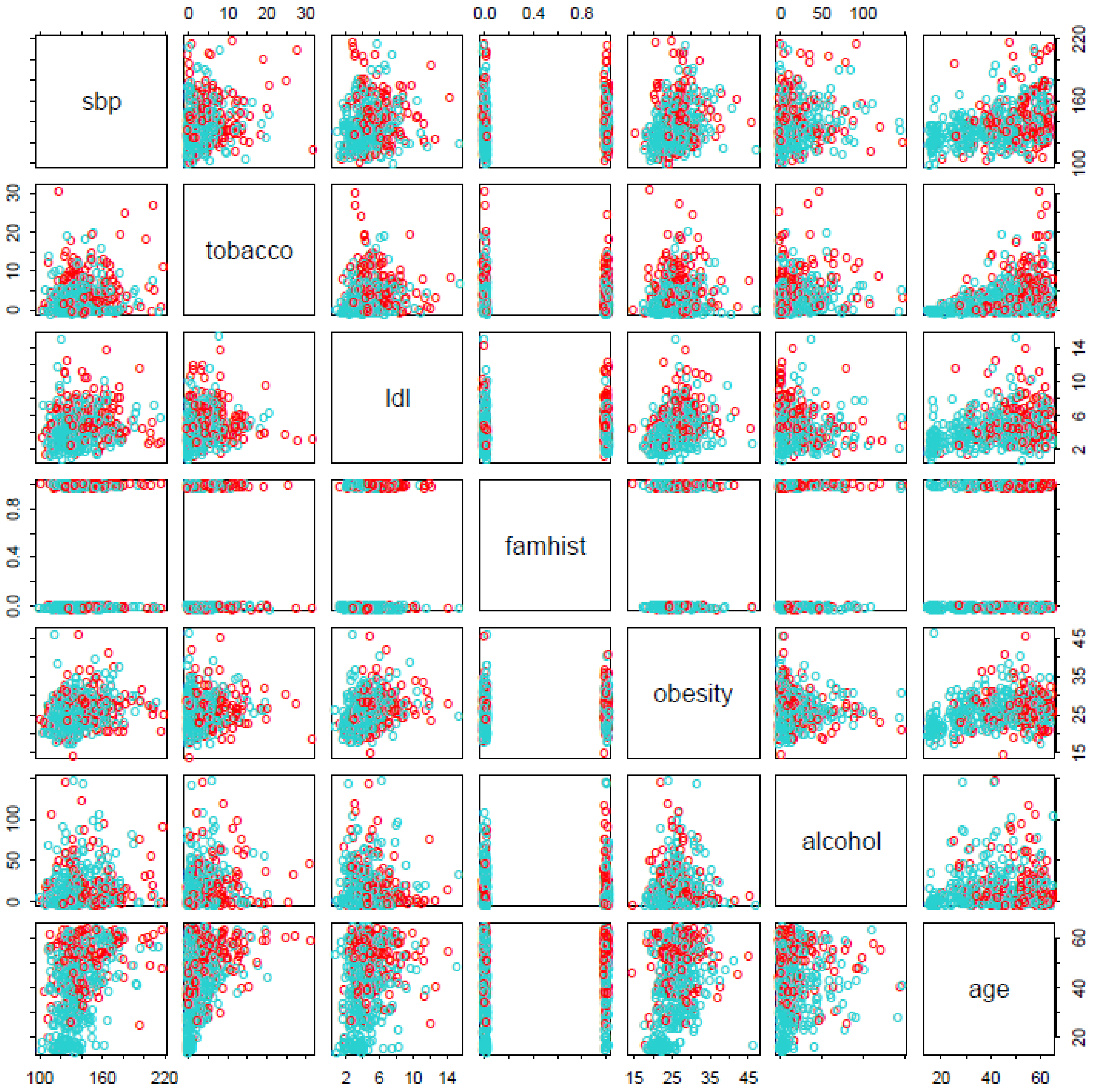
https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Using Logistic Regression

The role of Logistic Regression differs in ML and Data Science,

- In Machine Learning we use Logistic Regression for building predictive classification models
- In Data Science we use it for understanding & interpreting how features relate to data classes / categories

Example South African Heart Disease (Hastie et al. 2001)
Data result from Coronary Risk-Factor Study in 3 rural areas of South Africa. Data are from white men 15-64yrs and response is presence/absence of *myocardial infraction (MI).* How predictive are each of the features?



Looking at Data

Each scatterplot shows pair of risk factors. Cases **with** MI (**red**) and **without** (**cyan**)

Features

- Systolic blood pressure
- Tobacco use
- Low density lipoprotein (ldl)
- Family history (discrete)
- Obesity
- Alcohol use
- Age

[Source: Hastie et al. (2001)]

Example: African Heart Disease

	Coefficient	Std. Error	Z Score
(Intercept)	−4.130	0.964	−4.285
sbp	0.006	0.006	1.023
tobacco	0.080	0.026	3.034
ldl	0.185	0.057	3.219
famhist	0.939	0.225	4.178
obesity	-0.035	0.029	−1.187
alcohol	0.001	0.004	0.136
age	0.043	0.010	4.184

Finding Systolic blood pressure (sbp) is **not a significant predictor**

Obesity is not significant and negatively correlated with heart disease in the model

Remember All correlations / significance of features are based on presence of *other features*. We must always consider that features are strongly correlated.

Example: African Heart Disease

	Coefficient	Std. Error	Z score
(Intercept)	−4.204	0.498	−8.45
tobacco	0.081	0.026	3.16
ldl	0.168	0.054	3.09
famhist	0.924	0.223	4.14
age	0.044	0.010	4.52

Doing some feature selection we find a model with 4 features: tobacco, ldl, family history, and age

How to interpret coefficients? (e.g. tobacco → 0.081)

$$\ln \frac{p(y=1 \mid x)}{p(y=0 \mid x)} = w^T x$$

- Tobacco is measured in total lifetime usage (in kg)
- Thus, increase of 1kg of lifetime tobacco yields

$$\exp(0.081) = 1.084$$

Or 8.4% increase in odds of coronary heart disease

- 95% CI is 3% to 14% since $\exp(0.081 \pm 2 \times 0.026) = (1.03, 1.14)$

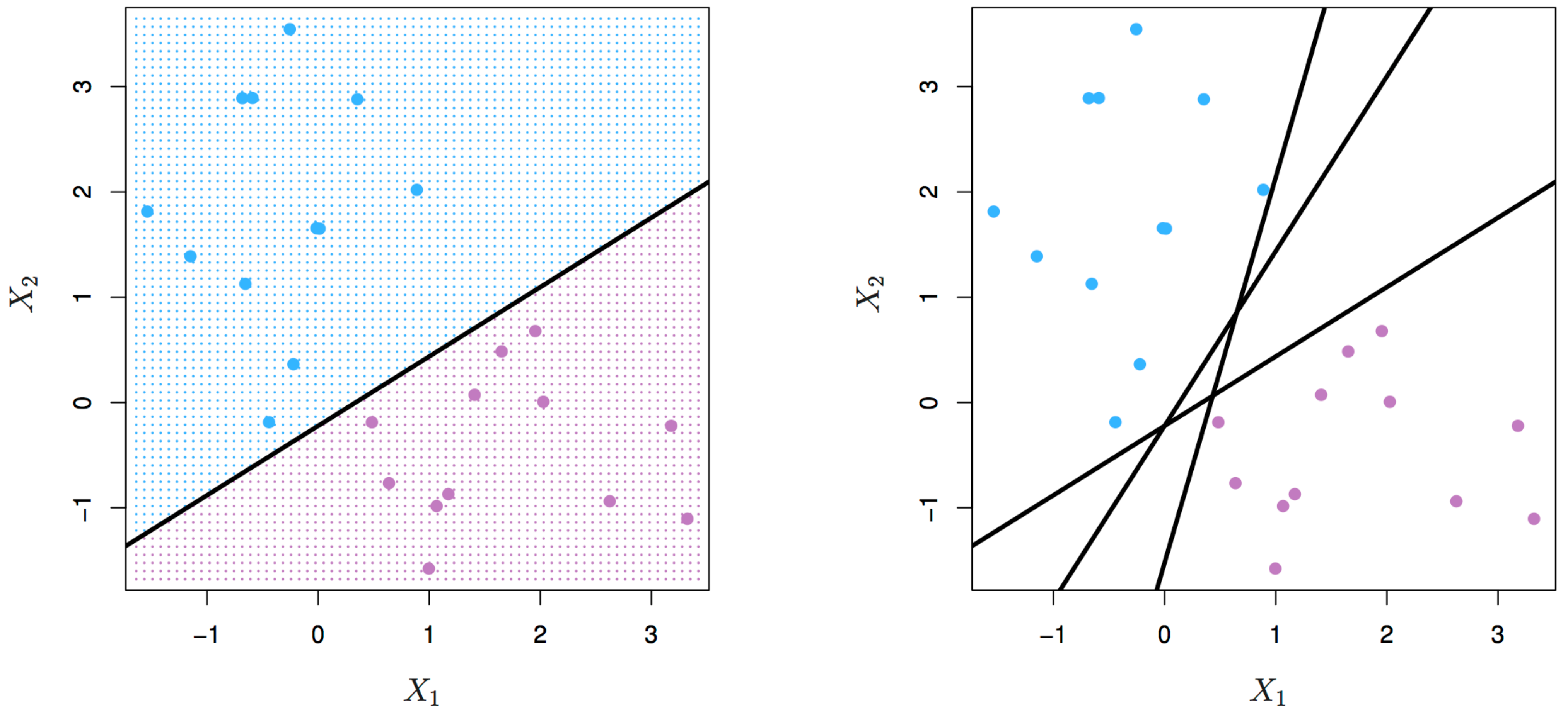
Outline

- Linear Models for Regression
  - Least Squares Estimation
  - Regularized Least Squares
- Linear Models for Classification
  - Logistic Regression
  - Support Vector Machine

Linear Decision Boundary

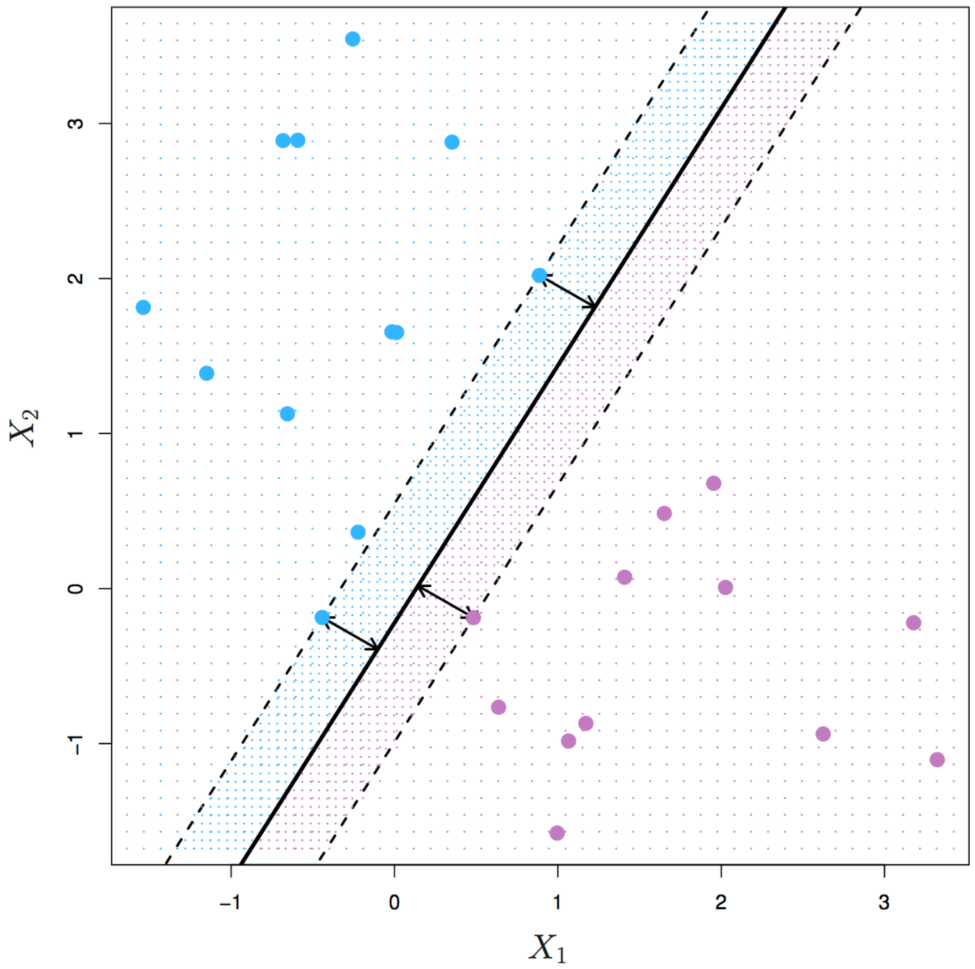
Any boundary that separates classes is equivalently good on training data

Are they equally good on unseen test data?



[Source: http://www-bcf.usc.edu/~gareth/ISL/]

Classifier Margin



*The **margin** measures minimum distance between each class and the decision boundary*

Observation Decision boundaries with larger margins are more likely to generalize to unseen data

Idea Learn the classifier with the largest margin that still separates the data…

…we call this a *max-margin classifier*

[Source: http://www-bcf.usc.edu/~gareth/ISL/]

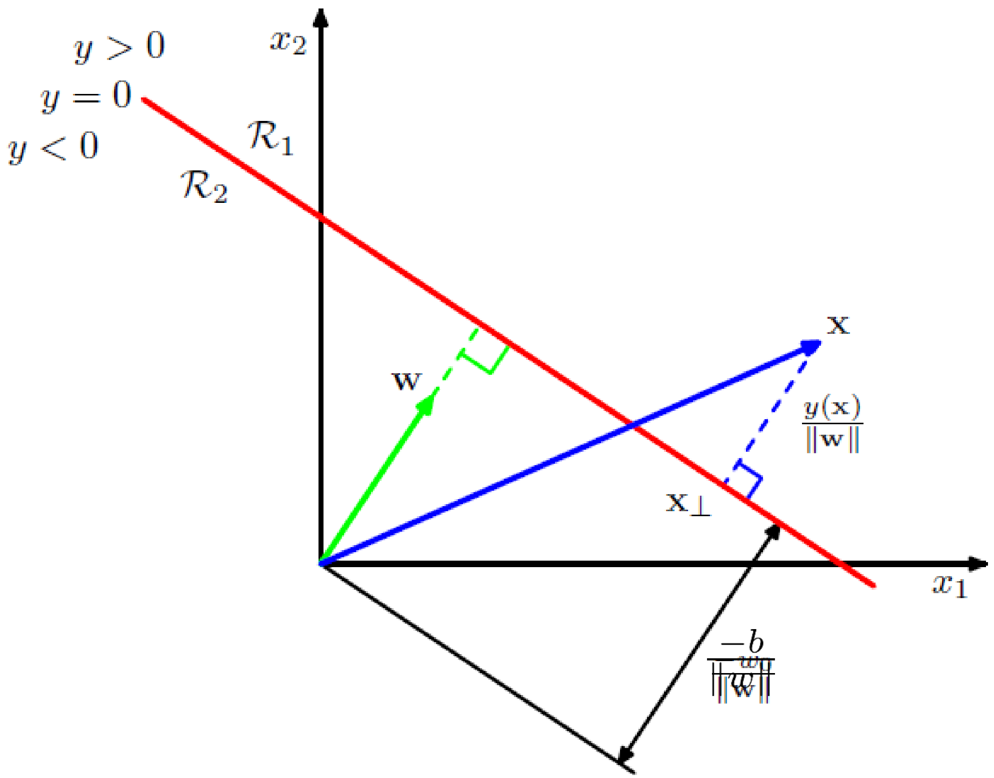
Max-Margin Classifier

Recall that the linear model is given by

$$f(x) = w^T x + b$$

Let classes be $\{-1, 1\}$ so classification rule is,

$$h(x) = \begin{cases} -1 & \text{if } f(x) < 0 \\ 1 & \text{if } f(x) \geq 0 \end{cases}$$



Decision boundary is now at $f(x) = 0$ and distance of x to it is:

$$\frac{f(x)}{\|w\|}$$

Known as the *distance from a point to a plane* equation:
[wiki/Distance_from_a_point_to_a_plane]

Where the norm of the weights is $\|w\| = \sqrt{w^T w} = \sqrt{\sum_i w_i^2}$

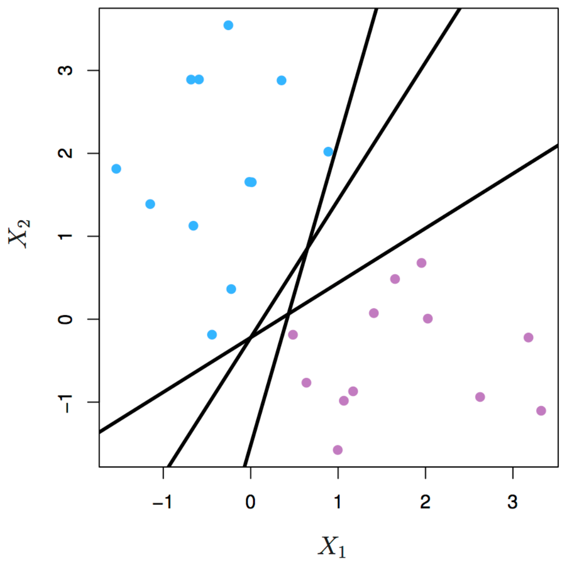
Max-Margin Classifier

For training data $\{(x_n, y_n)\}$, we would like to choose (w, b) to ensure two properties:

(1) all points are correctly classified:

$$y_n\,(w^\top x_n + b) > 0,\ n = 1, \dots N$$

(2) the margins of all points $\frac{|w^\top x_n + b|}{\|w\|}$, $n = 1, \dots N$ are as large as possible



This motivates the following optimization problem (O1):

$$\underset{w.b}{\text{maximize}}\ \left(\min_n \frac{|w^\top x_n + b|}{\|w\|}\right)$$

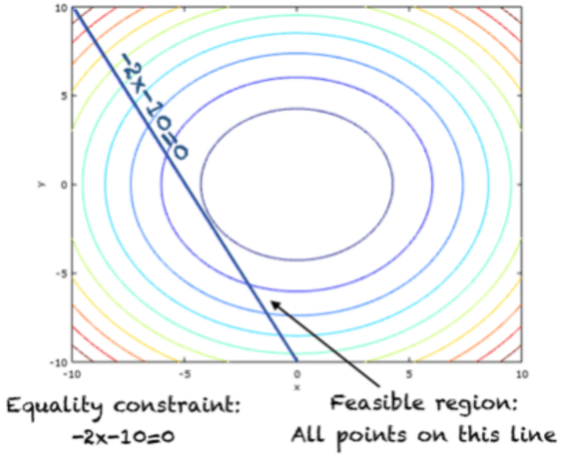
$$\text{subject to: } y_n\,(w^\top x_n + b) > 0,\ n = 1, \dots N$$

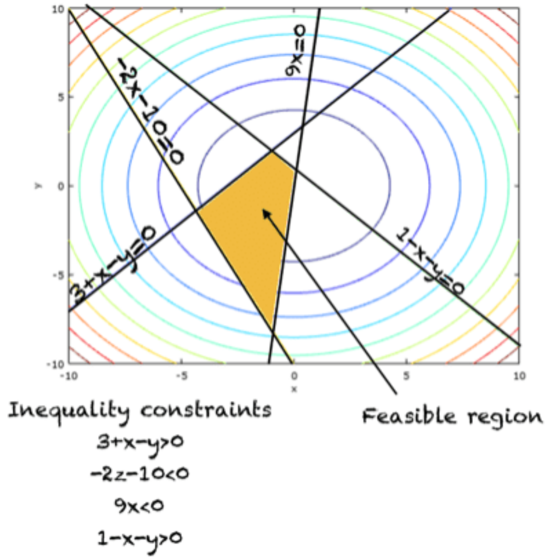
Constrained optimization

$$\min_{w} f(w)$$

$$s.t.\ g_i(w) \leq 0, \forall i = 1, \ldots, k \quad \text{(inequality constraints)}$$

$$h_j(w) = 0, \forall j = 1, \ldots, \ell \quad \text{(equality constraints)}$$





- When f is convex and

the constraint set is a convex set

=> convex optimization problem

=> efficient solvers abound

- Is (O1) a convex optimization problem?
- If not, can we convert it to one?

Max-Margin Classifier (cont'd)

(O1) $$\underset{w.b}{\text{maximize}} \left(\min_{n} \frac{|w^\top x_n + b|}{\|w\|} \right)$$ **Minimum margin**

$$\text{subject to: } y_n \left(w^\top x_n + b \right) > 0,\ n = 1, \ldots N$$ **Perfect classification**

- Note: under perfect classification, $\frac{|w^\top x_n + b|}{\|w\|} = \frac{y_n \left(w^\top x_n + b \right)}{\|w\|}$ for all n

- Therefore, (O1) is equivalent to (O2):

$$\underset{w.b}{\text{maximize}} \left(\min_{n} \frac{y_n \left(w^\top x_n + b \right)}{\|w\|} \right)$$

$$\text{subject to: } y_n \left(w^\top x_n + b \right) > 0,\ n = 1, \ldots N$$

Max-Margin Classifier

- (O2):

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{y_n\left(w^\top x_n + b\right)}{\|w\|} \right)$$

$$\text{subject to: } y_n\left(w^\top x_n + b\right) > 0,\ n = 1, \ldots N$$

- Infinitely many solutions – if (w, b) is optimal, then $(2w, 2b)$ is also optimal (for example)

- Break ties: add the constraint that $\min_n y_n\left(w^\top x_n + b\right) = 1$
- To solve (O2), it suffices to solve (O3):

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{y_n\left(w^\top x_n + b\right)}{\|w\|} \right)$$

$$\text{subject to: } \min_n y_n\left(w^\top x_n + b\right) = 1$$

SVM derivation (3)

(O3)
$$\max_{w,b} \min_{i=1}^{n} \frac{y_i(w^\top x_i + b)}{\|w\|}$$
$$s.t.\ \min_i y_i(w^\top x_i + b) = 1$$

- Summary: the constraint encodes (1) correct classification (2) there are no two solutions that represent the same hyperplane!
  - Note: If (w, b) is a solution, then the minimum margin is $\frac{1}{\|w\|}$

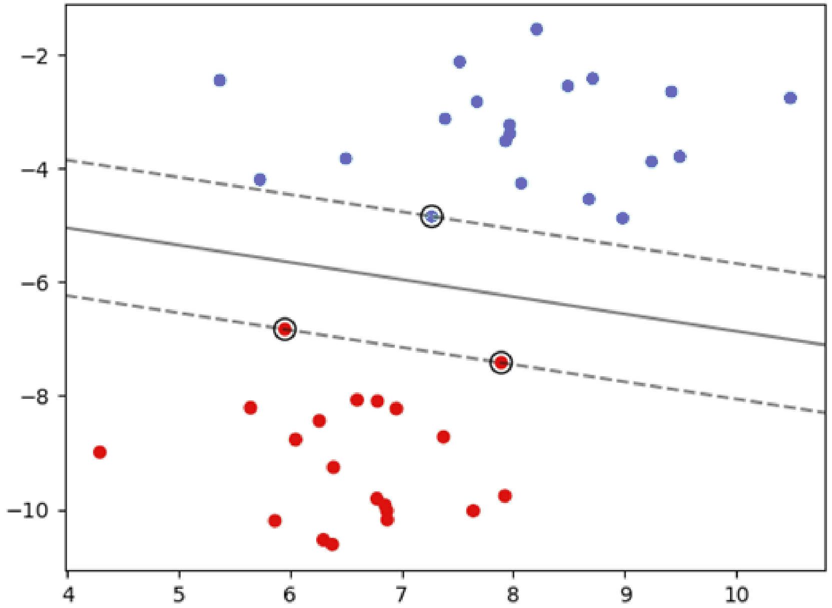
$$\max_{w,b} \frac{1}{\|w\|} \quad s.t.\ \min_i y_i(w^\top x_i + b) = 1 \quad \Leftrightarrow \quad \max_{w,b} \frac{1}{\|w\|} \quad s.t.\ \min_i y_i(w^\top x_i + b) \geq 1 \quad \Leftrightarrow \quad \max_{w,b} \frac{1}{\|w\|} \quad s.t.\ y_i(w^\top x_i + b) \geq 1, \forall i$$

(turns out to be equivalent..)

Final formulation in the linearly separable setting:
$$\min_{w,b} \|w\|^2$$
$$\text{s.t.}\ y_i(w^\top x_i + b) \geq 1, \forall i$$

Support Vector Machine (Primal)

To learn the classifier, we solve the following *constrained optimization problem…*



$$\text{minimize } \frac{1}{2}\|w\|^2$$
$$\text{subject to}$$
$$y_n(w^T x_n + b) \geq 1 \qquad \text{for } n = 1, \ldots, N$$

This is known as the *primal* optimization

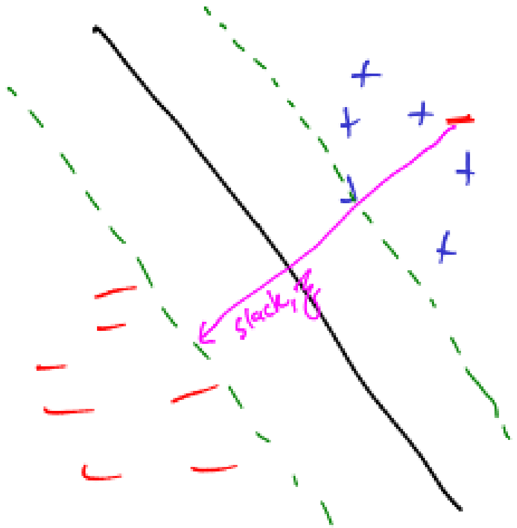
This is a convex optimization problem that can be solved efficiently

Why? check back "constrained optimization" slide

- Data are D-dimensional *vectors*
- Margins determined by nearest data points called *support vectors*
- We call this a *support vector machine* (SVM)

SVM in the nonseparable setting: Soft-margin

$$\min_{w,b} \|w\|^2$$
$$s.t.\;\; y_i(w^\top x_i + b) \geq 1, \forall i$$

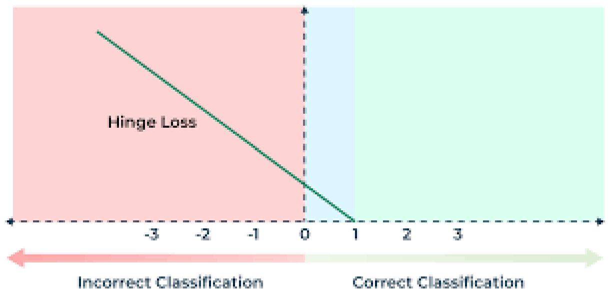


- What if data are **not** linearly separable?
- Introduce 'slack' variables

$$\min_{w,b,\{\xi_i \geq 0\}} \|w\|^2 + C\sum_{i=1}^{n} \xi_i \qquad \text{// } C \text{ is a hyper-parameter}$$
$$s.t.\;\; y_i(w^\top x_i + b) \geq 1 - \xi_i, \forall i$$

- Again, a convex optimization problem
- Fix any w, b, what is the optimal ξ?

$\xi_i = 0$ if $y_i(w^\top x_i + b) \geq 1$, and $\xi_i = 1 - y_i(w^\top x_i + b)$ otherwise

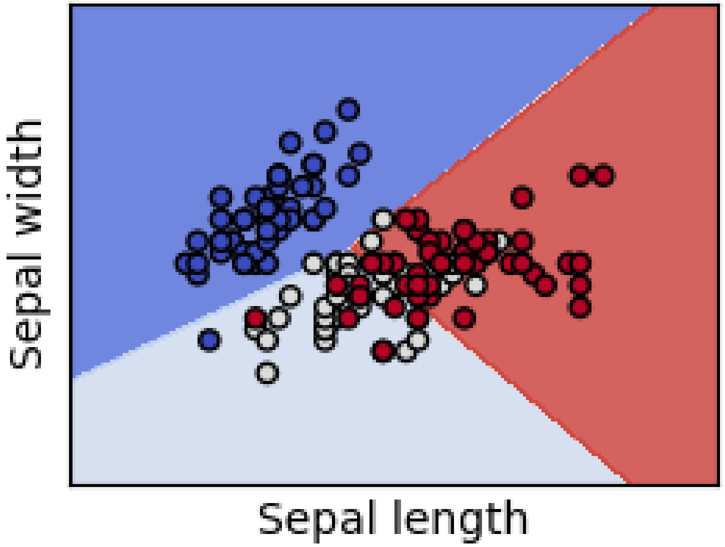


$$\min_{w,b} \|w\|^2 + C\sum_{i=1}^{n} \left(1 - y_i(w^\top x_i + b)\right)_+ \quad \Leftrightarrow \text{Regularized hinge loss minimization}$$

SVM in Scikit-Learn

SVM with linear decision boundaries,

[sklearn.svm.LinearSVC]



Call options include…

penalty : *{'l1', 'l2'}, default='l2'*

Specifies the norm used in the penalization. The 'l2' penalty is the standard used in SVC. The 'l1' leads to `coef_` vectors that are sparse.

dual : *bool, default=True*

Select the algorithm to either solve the dual or primal optimization problem. Prefer dual=False when n_samples > n_features.

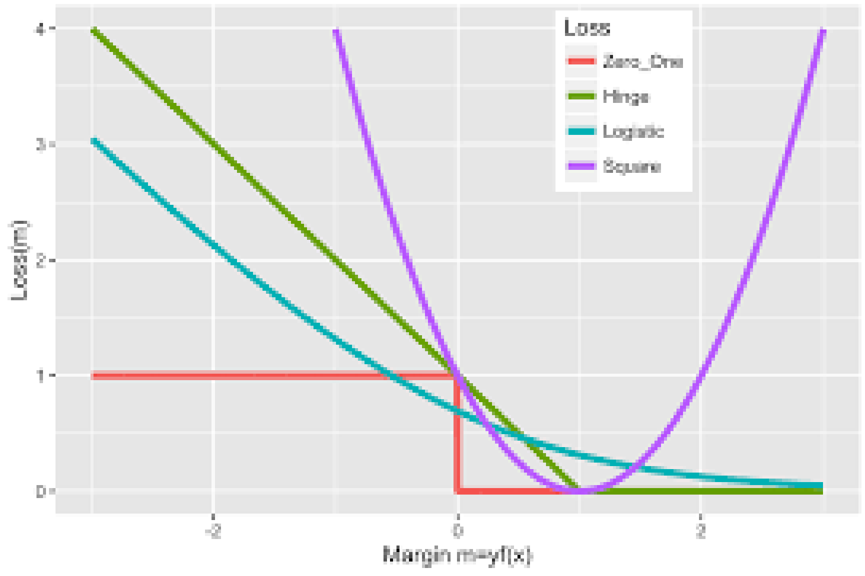
C : *float, default=1.0*

Regularization parameter. The strength of the regularization is inversely proportional to C. Must be strictly positive.

Other options for controlling optimizer (e.g. convergence tolerance 'tol')

Learning linear models: unified view

- All model training in this lecture can be viewed as **regularized loss minimization**



$$\hat{w} = \text{argmin}_{w \in \mathbb{R}^d} \sum_{i=1}^{n} \ell(w; x_i, y_i) + \lambda \, R(w)$$

- ℓ: loss function – logistic / hinge / square / ..
- R: regularizer – L1 / L2 / Lq / …

- Can oftentimes be optimized by (stochastic) gradient descent & friends very efficiently
  - E.g. see Allen-Zhu's ICML 2017 tutorial

Next lecture

- Nonlinear models: kernel methods

- Assigned reading: CIML Chap. 11

Backup

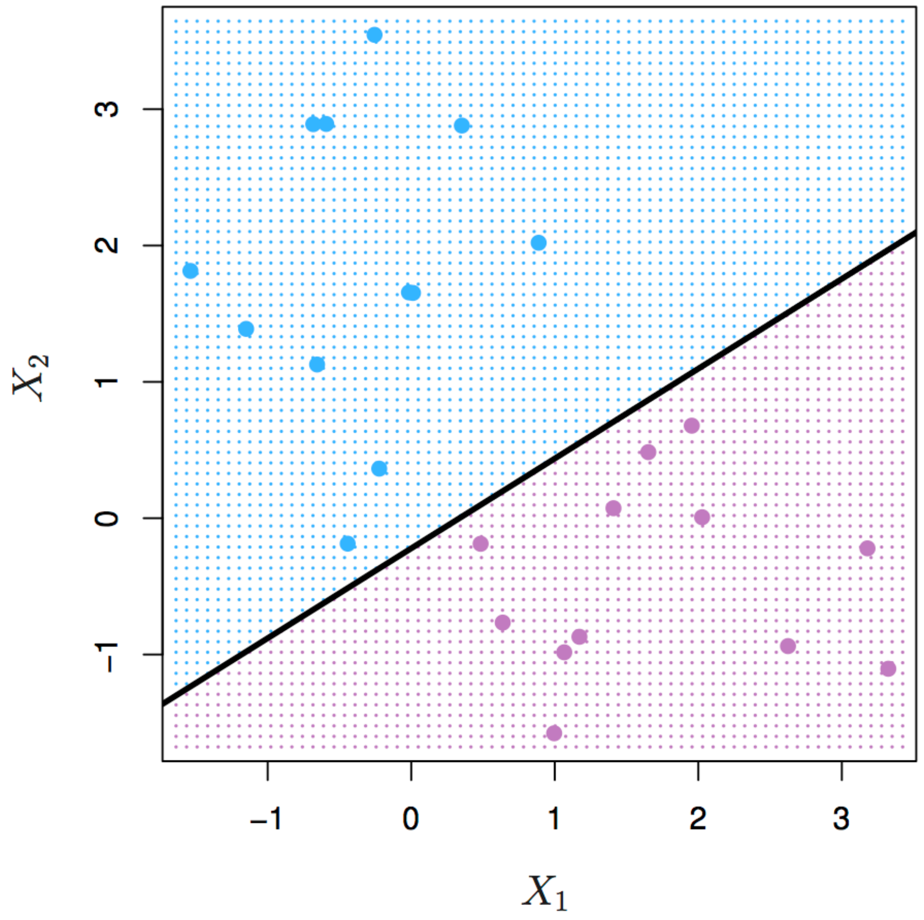
Next lecture

- Nonlinear models: kernel methods

- Assigned reading: CIML Chap. 11

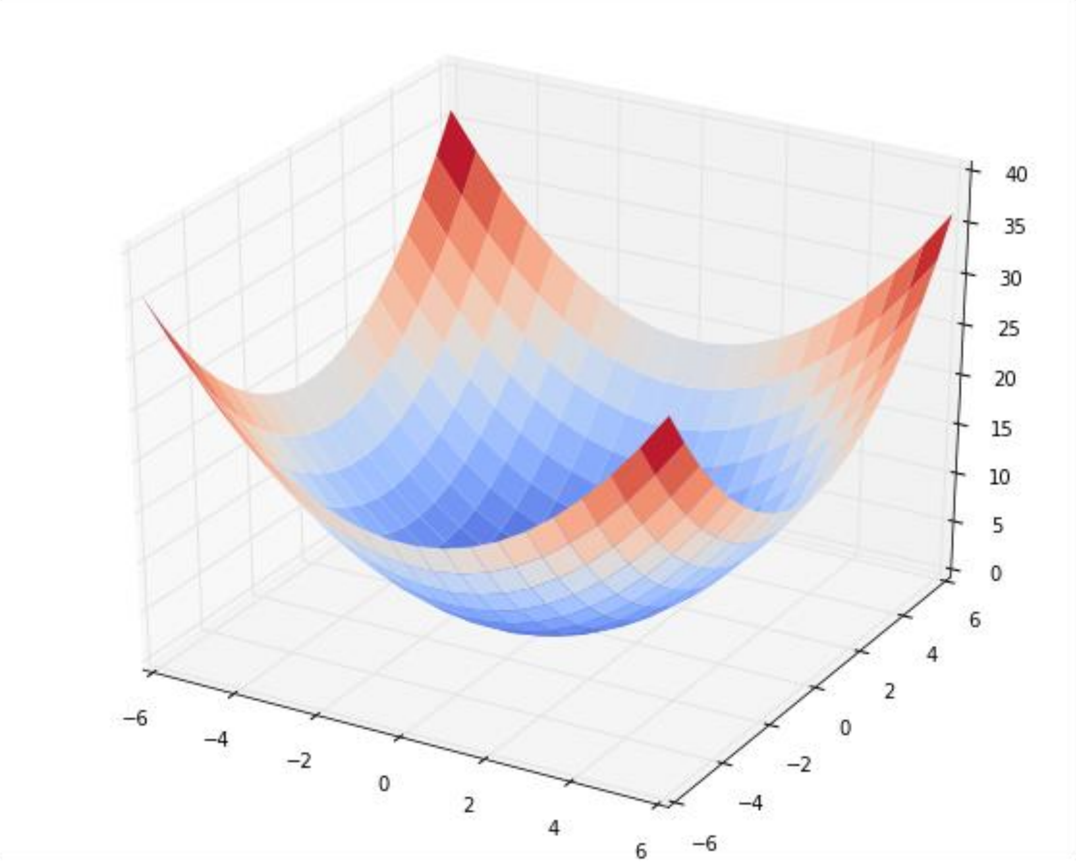
Linear Decision Boundary

Least squares regression yields decision boundary based on least squares solution…



[Source: http://www-bcf.usc.edu/~gareth/ISL/]

Multivariate Quadratic Form



Quadratic form for vectors is given by inner product,

$$\frac{1}{2\sigma^2}(y-\mu)^T(y-\mu)$$

For iid data MLE of Gaussian mean is once-again least squares,

$$\min_{\mu} \sum_{i=1}^{N} (y_i - \mu)^2$$

- Strongly convex
- Differentiable
- Unique optimizer at zero gradient

Notation

Substitute multi-dimensional linear regression…

$$p(y \mid \mu) = \mathcal{N}(y \mid \mu, \sigma^2)$$

$$p(y \mid w, x) = \mathcal{N}(y \mid w^T x, \sigma^2 I)$$

…brings us back to the least squares solution

Pseudoinverse

$$w^{\mathrm{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

The *Moore-Penrose pseudoinverse* is denoted,

$$X^\dagger = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$$

- Generalization of the standard matrix inverse
- Exists even for non-invertible X^TX
- Directly computable in most libraries
- In Numpy it is: `linalg.pinv`

Notes on L2 Regularization

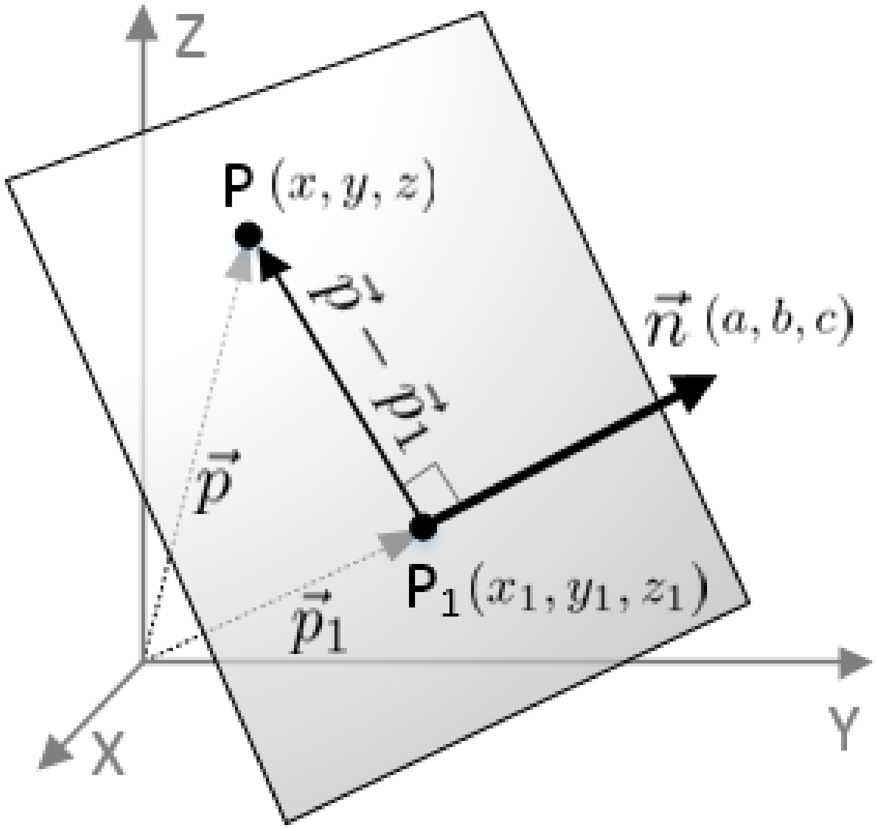
- Feature weights are "shrunk" towards zero (and each other) – statisticians often call this a "shrinkage" method
- Typically do **not** penalize bias (y-intercept, w_0) parameter,

$$\min_w \sum_i (y_i - w^T x_i - w_0)^2 + \lambda \sum_{d=1}^{D} w_d^2$$

- Penalizing w_0 would make– adding a constant c to Y would **not** add a constant to solution weights
- Can fit bias in a two-step procedure, by *centering* features $x_{ij} - \bar{x}$ then bias estimate is $w_0 = \bar{y}$
- Solutions are **not** invariant to scaling, so typically we standardize (e.g. Z-score) features before fitting model (Sklearn `StandardScaler`)

Moving to higher dimensions…

In higher dimensions Line → Plane



Multiple ways to define a plane, we will use:

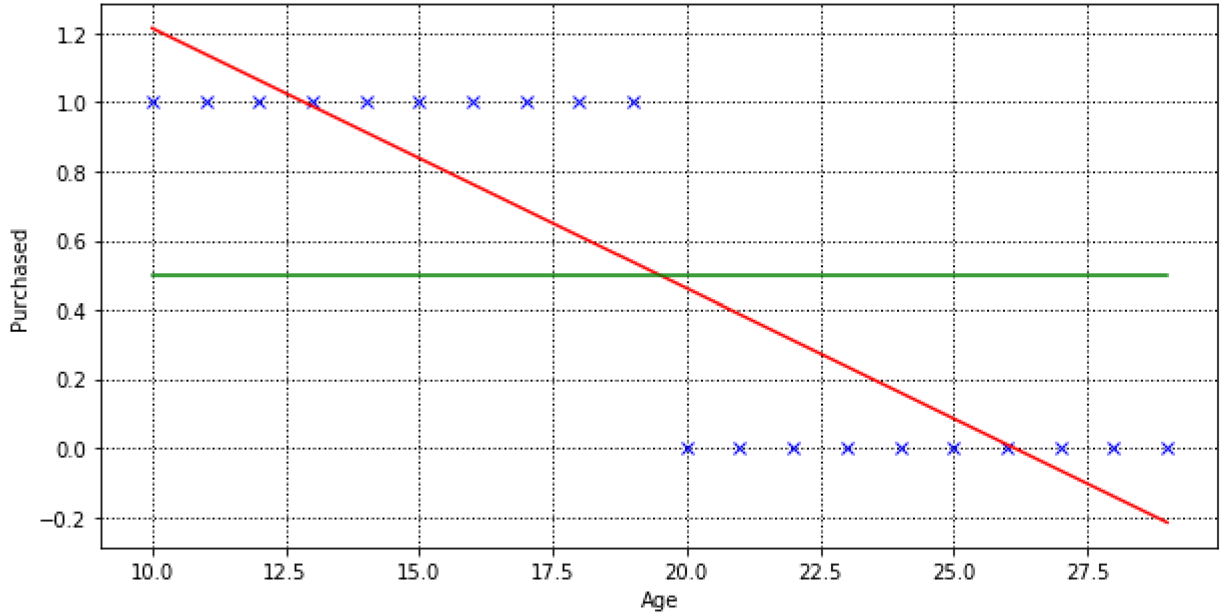
$$n^T(p - p_1) = 0$$

Normal Vector (controls orientation)

In-Plane Vector (handles offset)

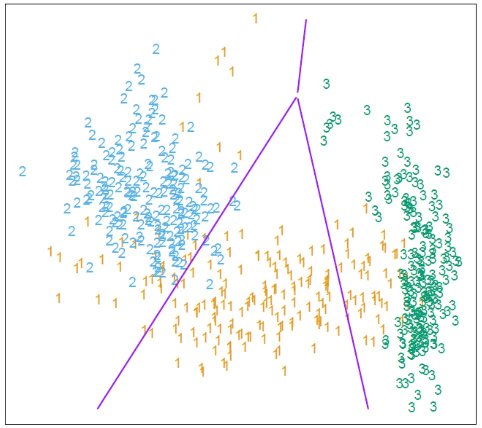
Source: http://www.songho.ca/math/plane/plane.html

Classification as Regression



Recall our linear regression can be used for classification via the rule,

$$\text{Class} = \begin{cases} 0 & \text{if } w^T x < 0.5 \\ 1 & \text{if } w^T x >= 0.5 \end{cases}$$

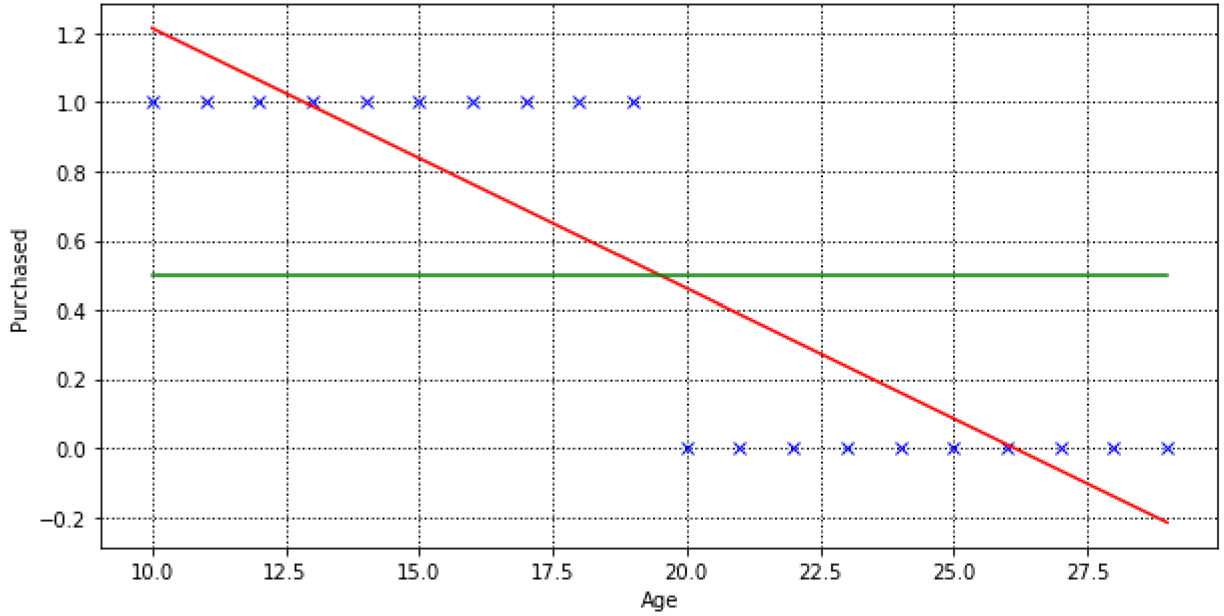


Generalizes to higher-dimensional features

- This is a *discriminant* function, since it discriminates between classes
- It is a linear function and so is a *linear discriminant*
- Green line is the *decision boundary* (also linear)

https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Classification as Regression



Idea Fit a least-square linear regressor *w* to the data (red). Classify points based on whether they are *above* or *below* the midpoint (green).

$$f(x) = \begin{cases} 0 & \text{if } w^T x < 0.5 \\ 1 & \text{if } w^T x \geq 0.5 \end{cases}$$

- This is a *discriminant* function, since it discriminates between classes
- It is a linear function and so is a *linear discriminant*
- We can call this approach **least squares classification**

https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Least squares classification: rationale

Recall: Bayes optimal classifier

$$f^*(x) = \begin{cases} 0 & \text{if } P(y = 1 \mid x) < 0.5 \\ 1 & \text{if } P(y = 1 \mid x) \geq 0.5 \end{cases}$$

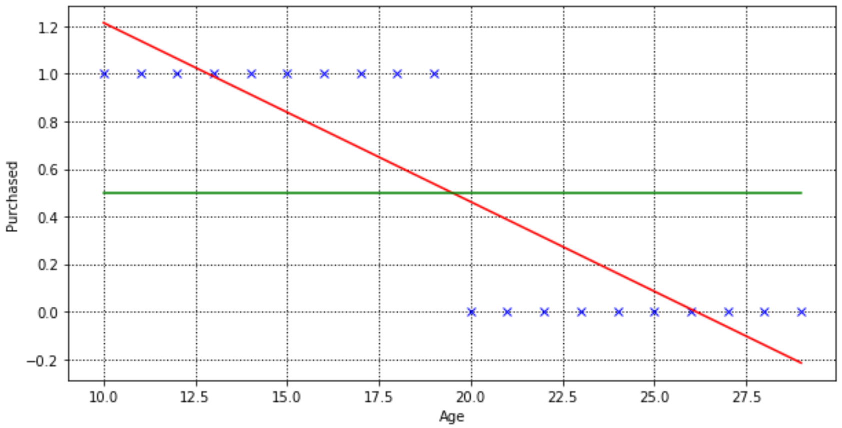
Recall the linear regression model, $p(y \mid x) = \mathcal{N}(w^T x, \sigma^2)$

So linear regression models the expected value,

$$w^T x \approx \mathbf{E}[y \mid x] = P(y = 1 \mid x)$$

$$f(x) = \begin{cases} 0 & \text{if } w^T x < 0.5 \\ 1 & \text{if } w^T x \geq 0.5 \end{cases}$$

Linear Probability Models



$$h(x) = I(w^T x \geq 0.5)$$

Binary Classification Linear model approximates probability of class assignment,

$$w^T x \approx p(y = 1 | x)$$

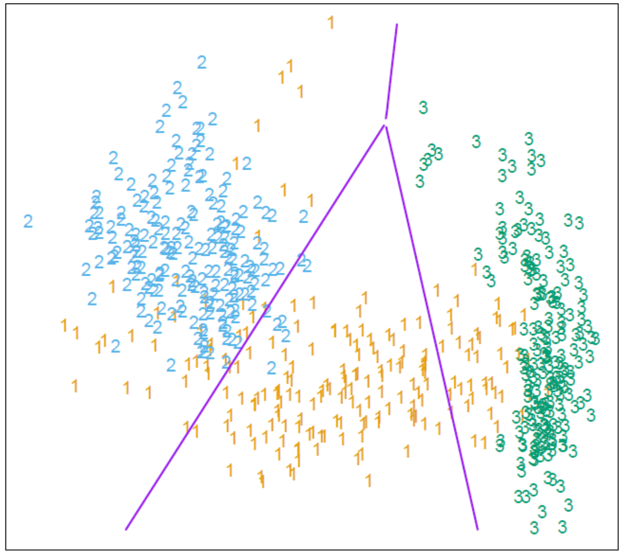
Multiclass Classification Multiple decision boundaries, each approximated by the class-specific linear model,

$$\hat{f}_k(x) = W_{k:} x$$

Where $W_{k:}$ is k[th] row

Approximates probability of class assignment,

$$\hat{f}_k(x) \approx p(y = k \mid x)$$



Notation

Likelihood of linear basic regression model…

$$p(y \mid w, x) = \mathcal{N}(y \mid wx, \sigma^2)$$

$$p(y \mid \mu) = \mathcal{N}(y \mid \mu, \sigma^2)$$

…we will just look at learning mean parameter for now

Multivariate Gaussian Distribution

We have only seen scalar (1-dimensional) X, but MLE is still least squares for higher-dimensional X…

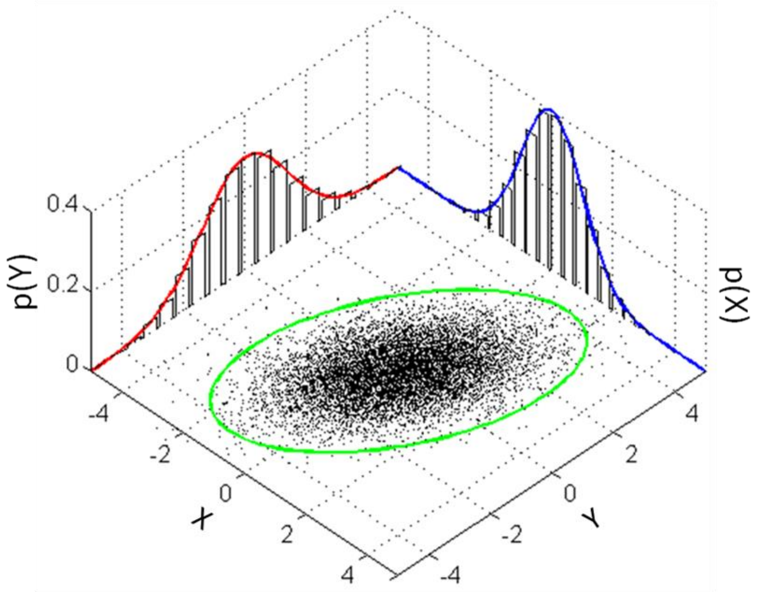
Let $X \in \mathcal{R}^d$ with mean $\mu \in \mathcal{R}^d$ and positive semidefinite covariance matrix $\Sigma \in \mathcal{R}^{d \times d}$ then the PDF is,

$$\mathcal{N}(x \mid \mu, \Sigma) = |2\pi\Sigma|^{-1/2} \exp -\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)$$

Again, the logarithm is a negative quadratic form,

$$\underbrace{\log |2\pi\Sigma|^{-1/2}}_{\text{Constant (in mean)}} - \underbrace{\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}_{\text{Quadratic Function of mean}}$$

Constant (in mean) **Quadratic Function of mean**



What's the rational?

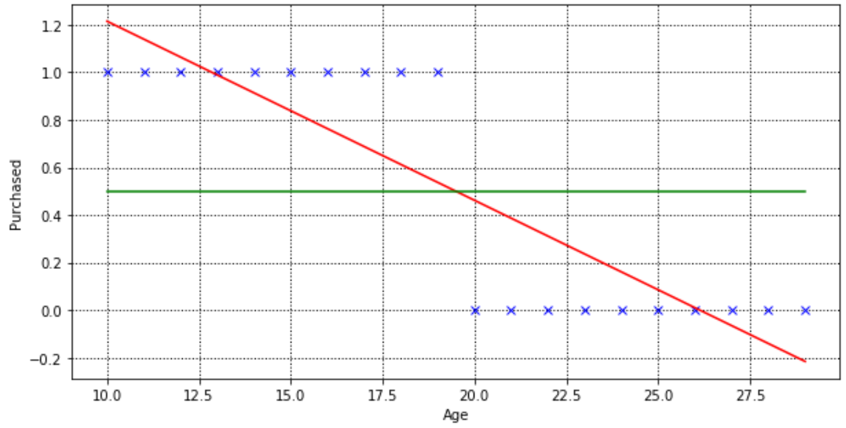
For *discrete* values we have that,

$$\mathbf{E}[y_k \mid x] = f_k(x) = p(\text{Class} = k \mid x)$$

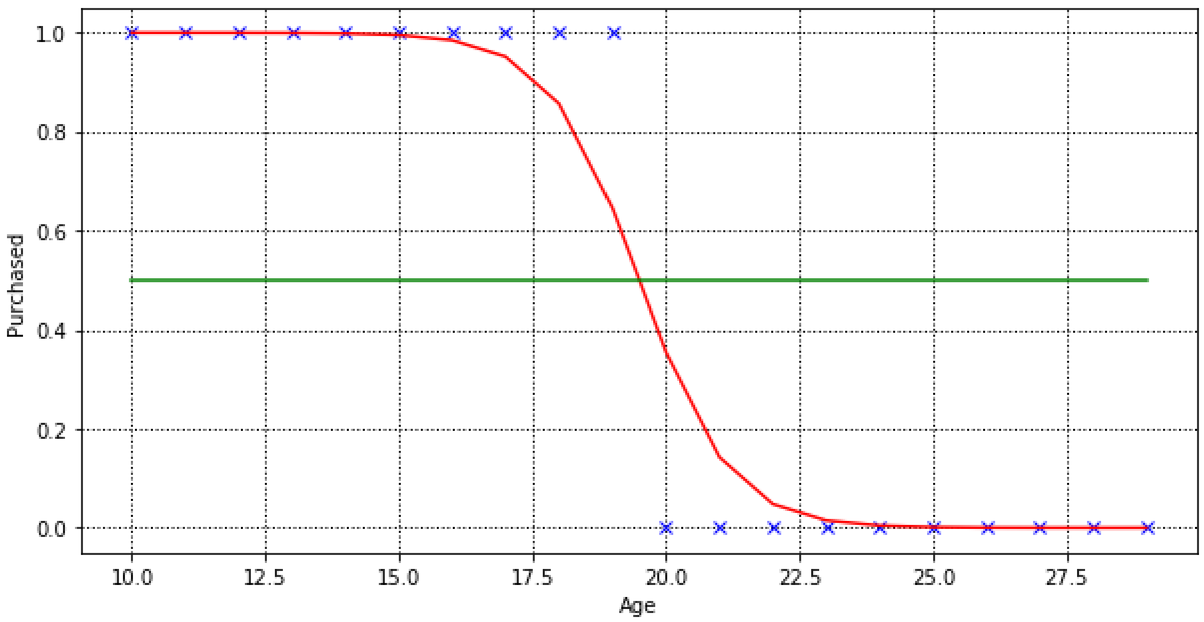
Can easily verify that they sum to 1,

$$\sum_{k=1}^{K} f_k(x) = 1$$

But they are not guaranteed to be positive!



Logistic Regression: Decision Boundary



Bayes optimal prediction:

predict 1 if $p(y = 1 \mid x) \geq 0.5$

$$\frac{p(C = 1 \mid x)}{p(C = 0 \mid x)}$$

If this ratio is greater than 1.0 then classify as C=1, otherwise C=0

In practice, we use the (natural) logarithm of the posterior odds ratio,

$$\log \frac{p(C = 1 \mid x)}{p(C = 0 \mid x)} = w^T x$$

This is a *linear decision boundary*

Logistic regression is a *linear classifier*

Iteratively Reweighted Least Squares

- Given some estimate of the weights w^{old} update by solving,

$$w^{\text{new}} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{z}$$

Design Matrix (NxD)

NxN Diagonal Weight matrix

Where z is the gradient direction,

$$\mathbf{z} = \mathbf{X} w^{\text{old}} + \mathbf{W}^{-1} (\mathbf{y} - \mathbf{p})$$

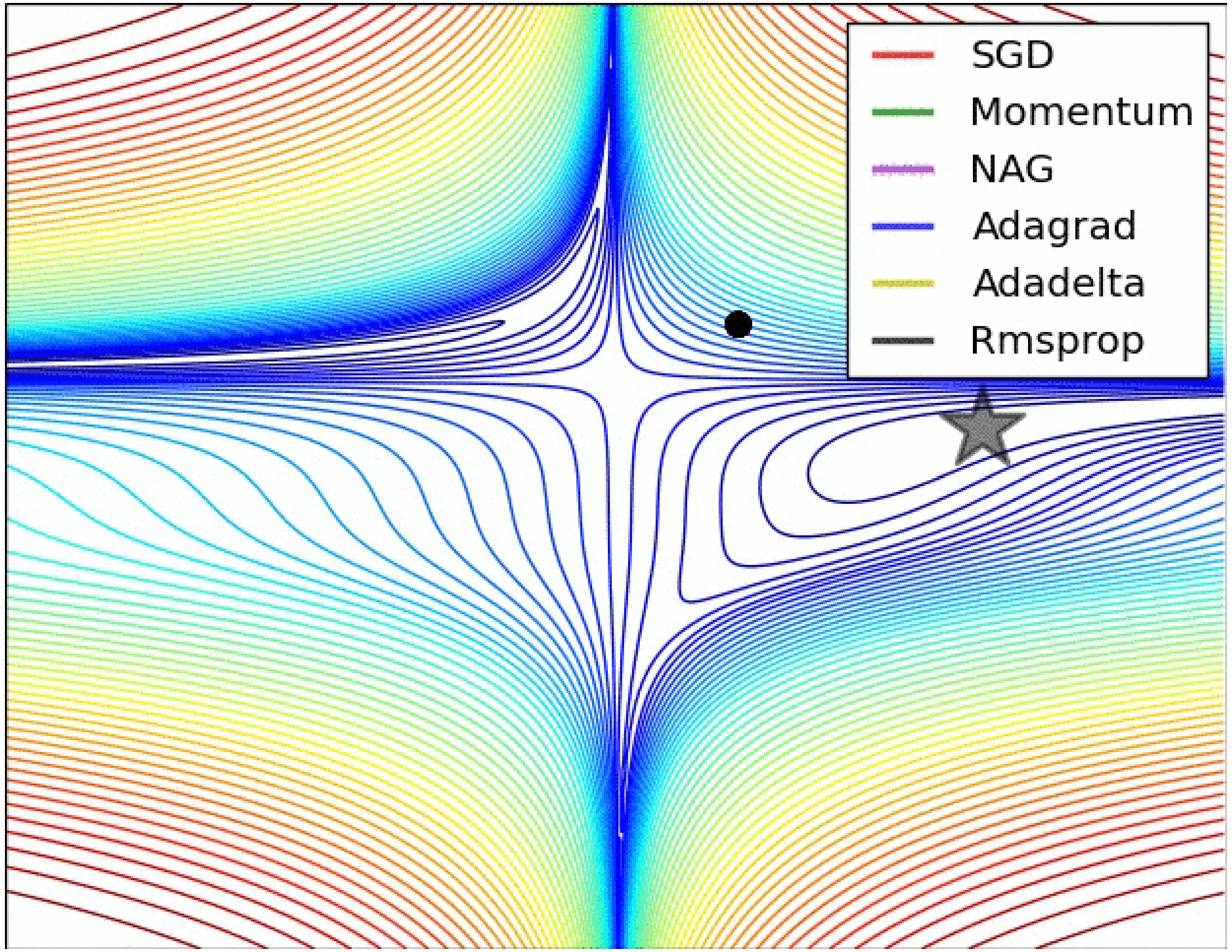
P(y=1|x) for each training point

- Essentially solving a *reweighted* version of least squares,

$$w^{\text{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Each iteration changes W and p so need to resolve

Choice of Optimizer



Since Logistic regression requires an optimizer, there are more parameters to consider

The choice of optimizer and parameters can affect time to fit model (especially if there are many features)

https://www.datasciencecentral.com/profiles/blogs/an-overview-of-gradient-descent-optimization-algorithms

Example: African Heart Disease

	Coefficient	Std. Error	Z Score
(Intercept)	−4.130	0.964	−4.285
sbp	0.006	0.006	1.023
tobacco	0.080	0.026	3.034
ldl	0.185	0.057	3.219
famhist	0.939	0.225	4.178
obesity	-0.035	0.029	−1.187
alcohol	0.001	0.004	0.136
age	0.043	0.010	4.184

Fit logistic regression to the data using MLE estimate via iterative reweighted least squares

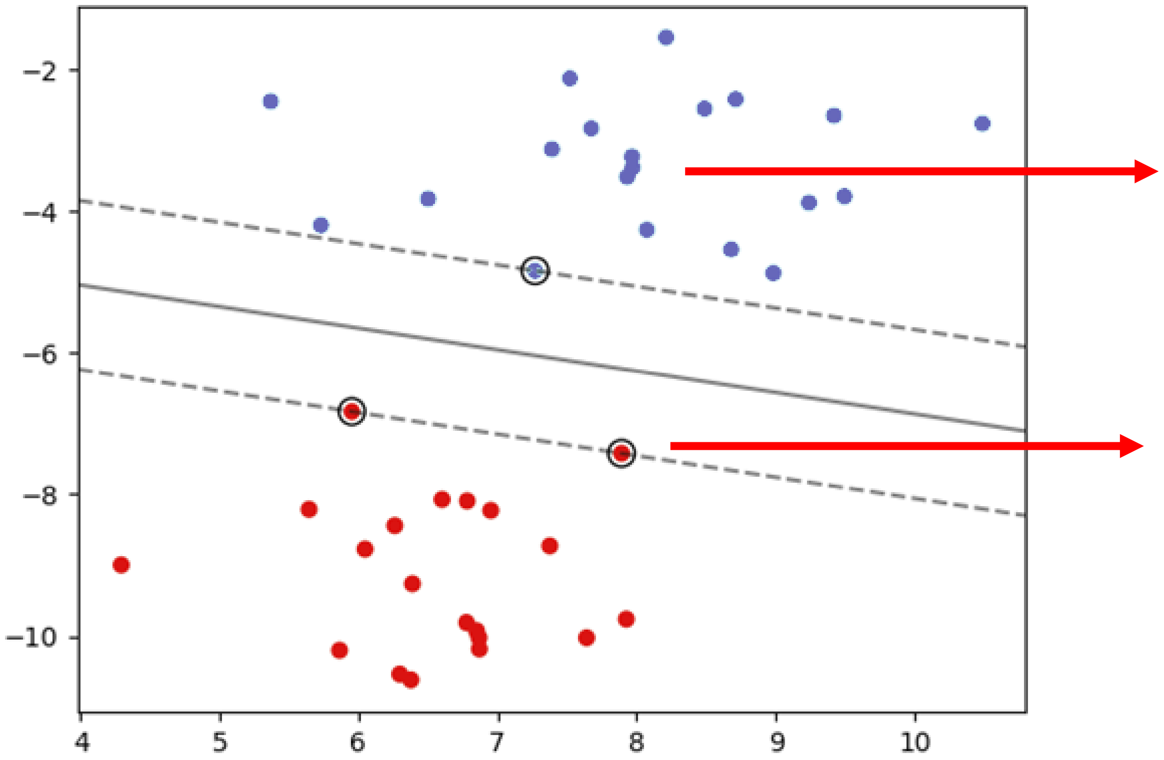
Standard error is estimated standard deviation of the learned coefficients

Recall, Z-score of weights is a random variable from standard Normal,

$$w_d \div \mathrm{SE}(w_d) \sim \mathcal{N}(0, 1)$$

Thus anything with Z-score > 2 is significant at 5% confidence level

Support Vector Machine (Dual)



All other points are outside the margin and constraints are *loose*:

$$y_n(w^T\phi(x_n)+b) > 1$$

Support vectors are tight to the margin, and satisfy constraints with equality:

$$y_n(w^T\phi(x_n)+b) = 1$$

SVM Dual Problem Find the support vectors (set of constraints that hold with equality) that define the largest margin

Max-Margin Classifier

For training data $\{(x_n, y_n)\}$ we only care about the margin for correctly-classified points where,

$$y_n y(x_n) = y_n(w^T x_n + b) > 0$$

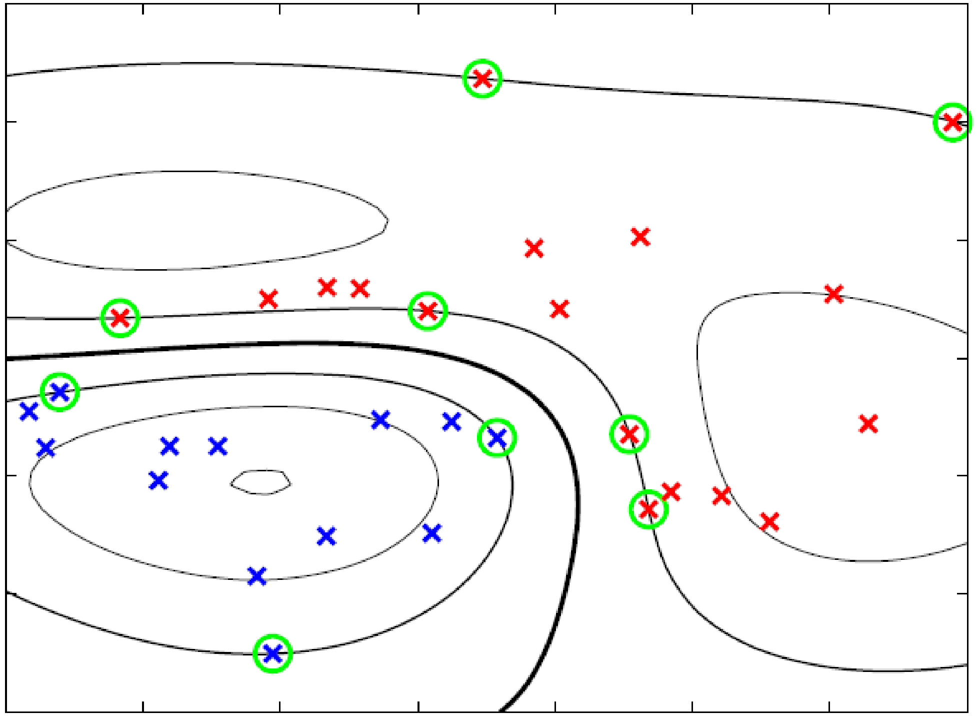
The margin of correctly-classified points is then given by,

$$\frac{y_n y(x_n)}{\|w\|} = \frac{y_n(w^T x_n + b)}{\|w\|}$$

Maximize margin over correctly-classified data points,

$$\arg\max_{w,b} \left\{ \min_n \frac{y_n(w^T x_n + b)}{\|w\|} \right\}$$

Nonlinear Max-Margin Classifier



Just as in the linear models we can introduce basis transformations,

$$y(x) = w^T \phi(x) + b$$

Max-margin learning is similar,

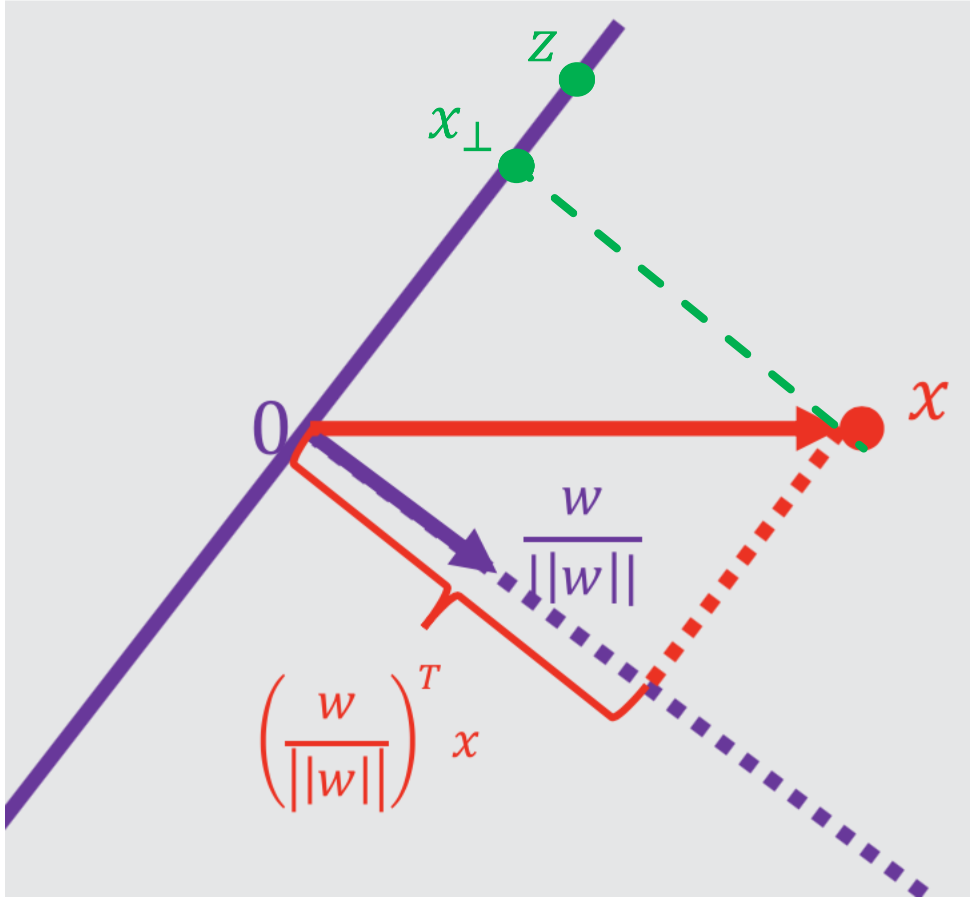
$$\arg\max_{w,b} \left\{ \min_n \frac{y_n(w^T \phi(x_n) + b)}{\|w\|} \right\}$$

Decision boundary is linear in the transformed data, but nonlinear in the original data space

[Source: Bishop, C. PRML]

Facts on vectors

- (Lem 1) a vector x has distance $\frac{w^\top x}{\|w\|}$ to the hyperplane $w^\top x = 0$

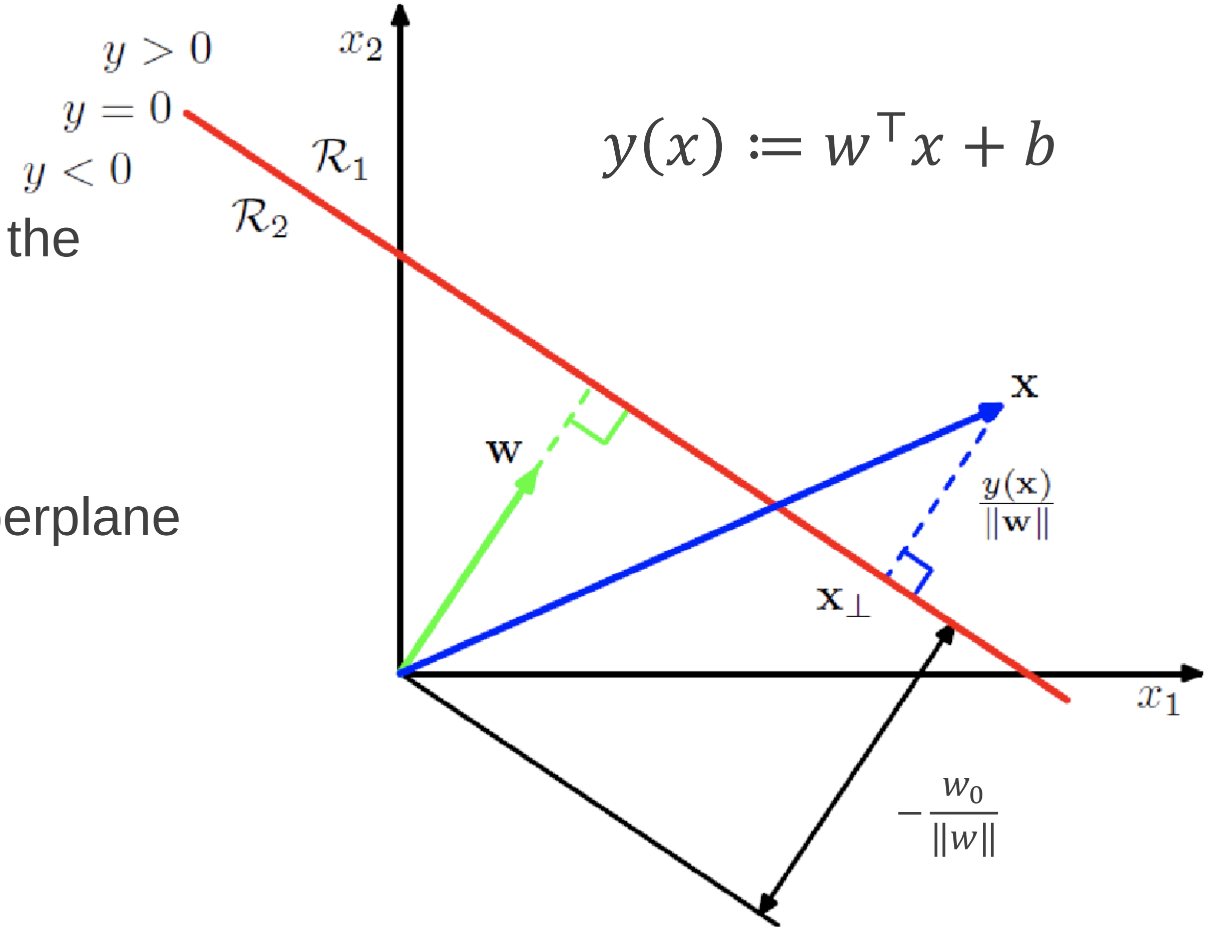


- How about with bias? $w^\top x + b = 0$
- Let us be explicit on the bias: $f(x; w, b) = w^\top x + b$

- recall: w is orthogonal to the hyperplane $w^\top x + b = 0$
  - why? (left as exercise)

Facts on vectors

- (Lem 2) x has distance $\frac{|w^\top x+b|}{\|w\|}$ to the hyperplane $w^\top x + b = 0$



$y(x) := w^\top x + b$

claim1 : x can be written as $x = x_\perp + r\frac{w}{\|w\|}$ where $x_\perp$ is the projection of x onto the hyperplane.

claim2 : then, $|r|$ is the distance between x and the hyperplane

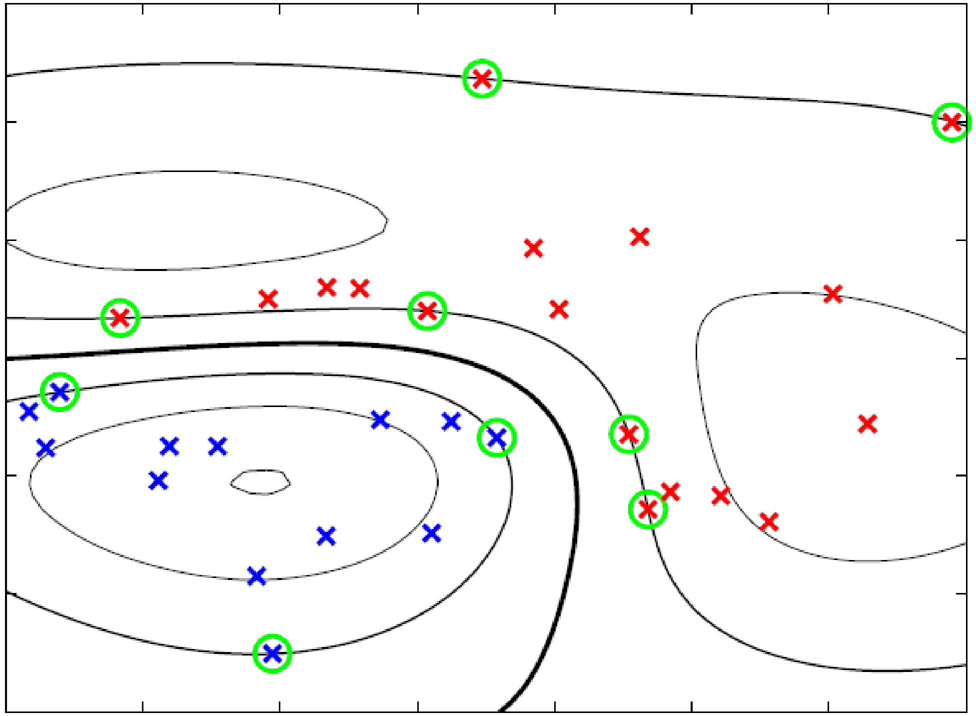
Solving for r: $w^\top x + b = w^\top x_\perp + r\frac{w^\top w}{\|w\|} + b = r\|w\|$.

this implies $|r| = \frac{|w^\top x+b|}{\|w\|}$

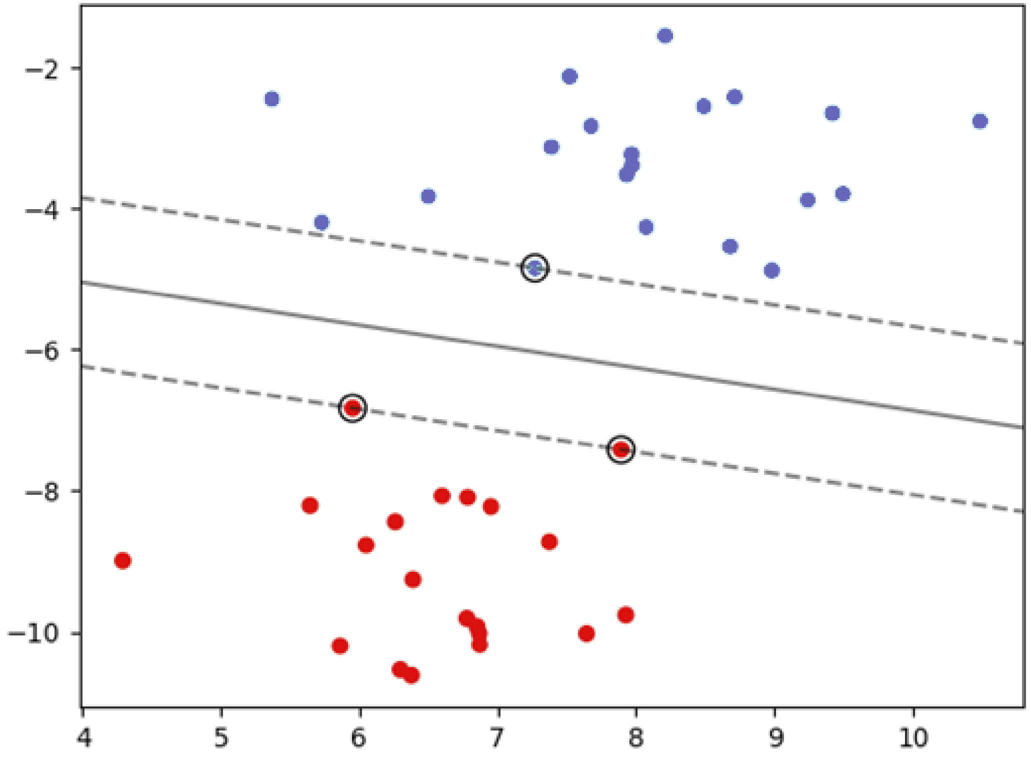
Figure from *Pattern Recognition and Machine Learning*, Bishop

Nonlinear Max-Margin Classifier

Data Space



Basis Space



Decision boundary is linear in the transformed data, but nonlinear in the original data space

Max-Margin Classifier

Learning objective is hard to solve in this form…

$$\arg\max_{w,b} \left\{ \min_n \frac{y_n(w^T\phi(x_n)+b)}{\|w\|} \right\}$$

But we can scale parameters $w \rightarrow \kappa w$ and $b \rightarrow \kappa b$ without changing margin…so we can set the nearest point to the margin so that,

$$y_n(w^T\phi(x_n)+b) = 1$$

And for all other points not near the margin,

$$y_n(w^T\phi(x_n)+b) \geq 1$$

Now we just have to satisfy these constraints…

SVM derivation (2)

- It's actually a matter of removing 'duplicates'; ∃ many (w,b)'s that actually represent the same hyperplane.

$$(\hat{w}, \hat{b}) = \max_{w,b} \min_{i=1}^{n} \frac{y_i(w^\top x_i + b)}{\|w\|}$$

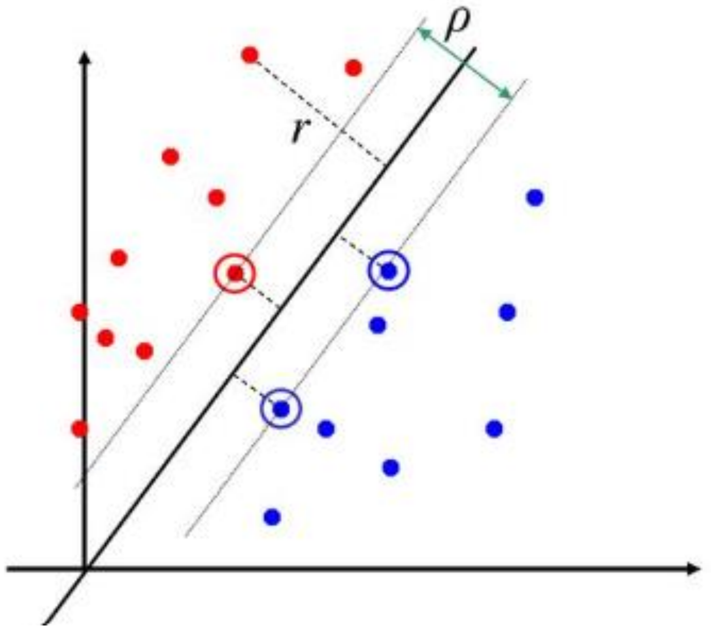
- Quick solution
  - For any solution $(\hat{w}, \hat{b})$, let x_{i^*} be the **closest to the hyperplane** $\hat{w} x_i + \hat{b} = 0$
  = achieves the smallest margin
  - Imagine rescaling $(\hat{w}, \hat{b})$ so that $\left|\hat{w}^\top x_{i^*} + \hat{b}\right| = 1$
- We can always do that, but can we find a formulation that automatically finds that modified solution?
  - add the constraint $\min_i y_i(w^\top x_i + b) = 1$

SVM derivation (1)

- Margin of (w, b) over all training points: $\gamma'(w,b) = \min_i \frac{|w^\top x_i + b|}{\|w\|}$

- Choose (w, b) with the maximum margin? .. wait, we also want it to be a perfect classifier
  - redefine it

$$\gamma(w,b) = \min_i \frac{y_i(w^\top x_i + b)}{\|w\|}$$



- Choose w with the maximum margin (and perfect classification)

$$(\hat{w}, \hat{b}) = \max_{w,b} \min_{i=1}^{n} \frac{y_i(w^\top x_i + b)}{\|w\|}$$

  - One more issue: still, infinitely many solutions..!

Max-Margin Classifier (cont'd)

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{|w^\top x_n + b|}{\|w\|} \right)$$ **Minimum margin**

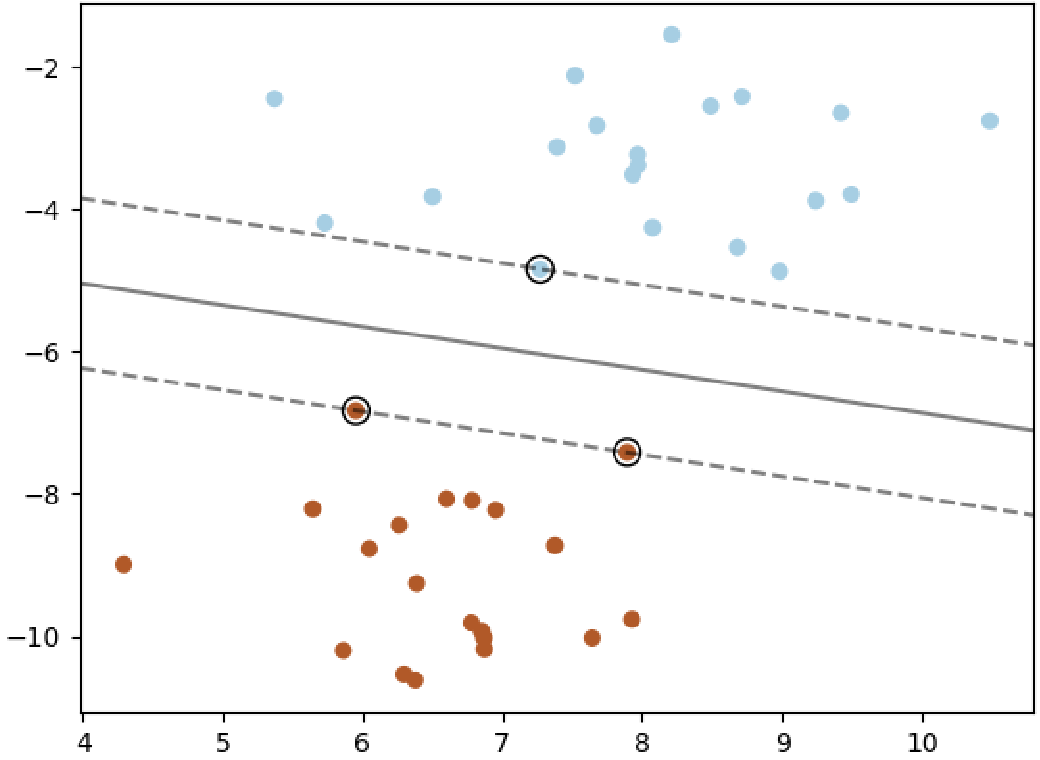
$$\text{subject to: } y_n\,(w^\top x_n + b) > 0,\ n = 1, \ldots N$$ **Perfect classification**

- Note: under perfect classification, $\frac{|w^\top x_n + b|}{\|w\|} = \frac{y_n\,(w^\top x_n + b)}{\|w\|}$

- Turns out: (O1) is equivalent to (O2):

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{y_n\,(w^\top x_n + b)}{\|w\|} \right)$$

Max-Margin Classifier



Maximize the minimum margin

$$\arg\max_{w,b} \left\{ \min_{n} \frac{y_n(w^T x_n + b)}{\|w\|} \right\}$$

Minimum margin over all training data

Find the parameters (w,b) that **maximize** the **smallest margin** over all the training data

[Source: http://www-bcf.usc.edu/~gareth/ISL/]

Max-Margin Classifier

- (O2):

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{y_n \left(w^\top x_n + b \right)}{\|w\|} \right)$$

- Infinitely many solutions – if (w, b) is optimal, then $(2w, 2b)$ is also optimal (for example)

- Break ties: add the constraint that $\min_n y_n \left(w^\top x_n + b \right) = 1$
- To solve (O2), it suffices to solve (O3):

$$\underset{w.b}{\text{maximize}} \left(\min_n \frac{y_n \left(w^\top x_n + b \right)}{\|w\|} \right)$$
$$\text{subject to: } \min_n y_n \left(w^\top x_n + b \right) = 1$$

SVM derivation (3)

(O3) $$\max_{w,b} \min_{i=1}^{n} \frac{y_i(w^\top x_i + b)}{\|w\|}$$
$$s.t.\ \min_i y_i(w^\top x_i + b) = 1$$

- Summary: the constraint encodes (1) correct classification (2) there are no two solutions that represent the same hyperplane!
  - Note: If $(\hat{w}, \hat{b})$ is a solution, then the margin is $\frac{1}{\|\hat{w}\|}$

$$\max_{w,b} \frac{1}{\|w\|} \quad s.t.\ \min_i y_i(w^\top x_i + b) = 1$$

$$\max_{w,b} \frac{1}{\|w\|} \quad s.t.\ \min_i y_i(w^\top x_i + b) \geq 1$$

(turns out to be equivalent..)

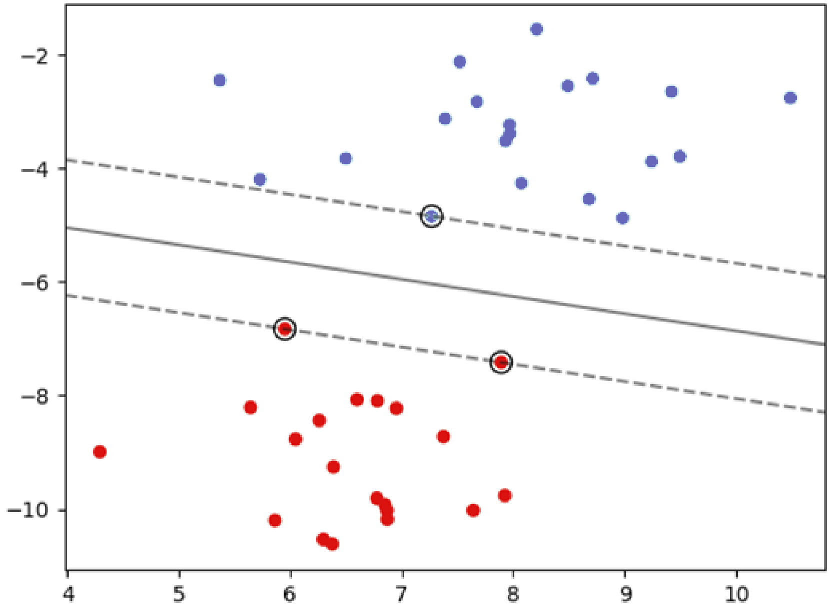
$$\max_{w,b} \frac{1}{\|w\|} \quad s.t.\ y_i(w^\top x_i + b) \geq 1, \forall i$$

Final formulation in the linearly separable setting:
(quadratic programming)

$$\min_{w,b} \|w\|^2$$
$$\text{s.t.}\ \ y_i(w^\top x_i + b) \geq 1, \forall i$$

Support Vector Machine (Primal)

To learn the classifier, we solve the following *constrained optimization problem…*



$$\text{minimize } \frac{1}{2}\|w\|^2$$
$$\text{subject to}$$
$$y_n(w^T x_n + b) \geq 1 \qquad \text{for } n = 1, \ldots, N$$

This is known as the *primal* optimization

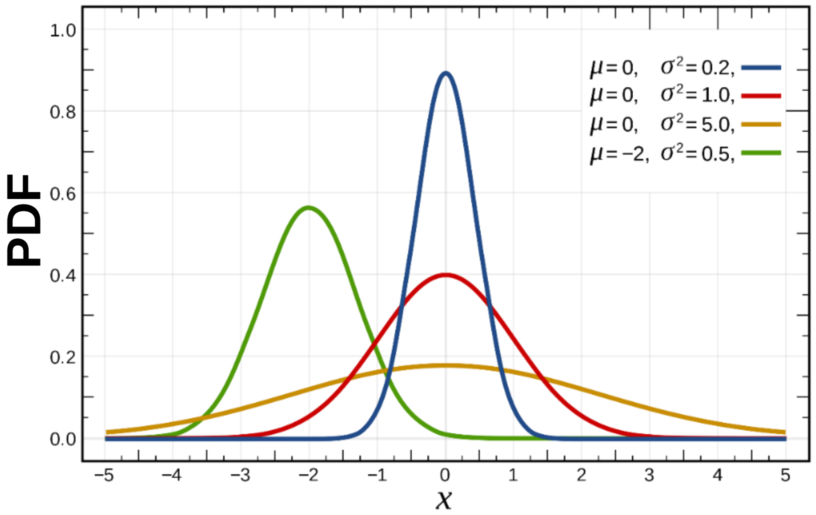
This is a convex (quadratic) optimization problem that can be solved efficiently

- Data are D-dimensional *vectors*
- Margins determined by nearest data points called *support vectors*
- We call this a *support vector machine* (SVM)

Univariate Gaussian (Normal) Distribution

Gaussian (a.k.a. Normal) distribution with mean (location) μ and variance (scale) σ^2 parameters,

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



The logarithm of the PDF is just a negative quadratic,

$$\log \mathcal{N}(x \mid \mu, \sigma^2) = -\frac{1}{2}\log 2\pi - \log\sigma - \frac{1}{2\sigma^2}(x-\mu)^2$$

Constant in mean — **Quadratic Function of mean**