Lecture 2: Linear models

Basics of modeling, optimization, and regularization

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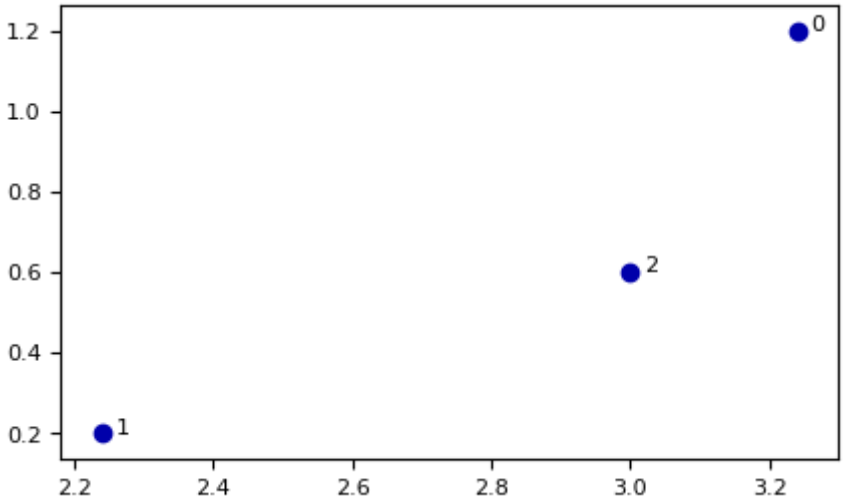
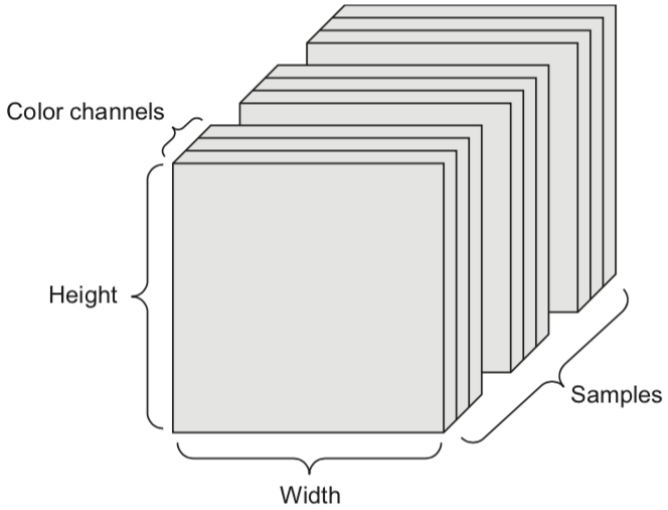
Notation and Definitions

- A *scalar* is a simple numeric value, denoted by an italic letter: $x = 3.24$
- A *vector* is a 1D ordered array of n scalars, denoted by a bold letter: $\mathbf{x} = [3.24, 1.2]$
  - x_i denotes the ith element of a vector, thus $x_0 = 3.24$.
    - Note: some other courses use $x^{(i)}$ notation
- A *set* is an *unordered* collection of unique elements, denote by caligraphic capital: $\mathcal{S} = \{3.24, 1.2\}$
- A *matrix* is a 2D array of scalars, denoted by bold capital: $\mathbf{X} = \begin{bmatrix} 3.24 & 1.2 \\ 2.24 & 0.2 \end{bmatrix}$
  - $\mathbf{X}_i$ denotes the ith *row* of the matrix
  - $\mathbf{X}_{:,j}$ denotes the jth *column*
  - $\mathbf{X}_{i,j}$ denotes the *element* in the ith row, jth column, thus $\mathbf{X}_{1,0} = 2.24$

- $\mathbf{X}^{n \times p}$, an $n \times p$ matrix, can represent n data points in a p-dimensional space
  - Every row is a vector that can represent a *point* in an n-dimensional space, given a *basis*.
  - The *standard basis* for a Euclidean space is the set of unit vectors
- E.g. if $\mathbf{X} = \begin{bmatrix} 3.24 & 1.2 \\ 2.24 & 0.2 \\ 3.0 & 0.6 \end{bmatrix}$



- A *tensor* is an k-dimensional array of data, denoted by an italic capital: T
  - k is also called the order, degree, or rank
  - $T_{i,j,k,...}$ denotes the element or sub-tensor in the corresponding position
  - A set of color images can be represented by:
    - a 4D tensor (sample x height x width x color channel)
    - a 2D tensor (sample x flattened vector of pixel values)



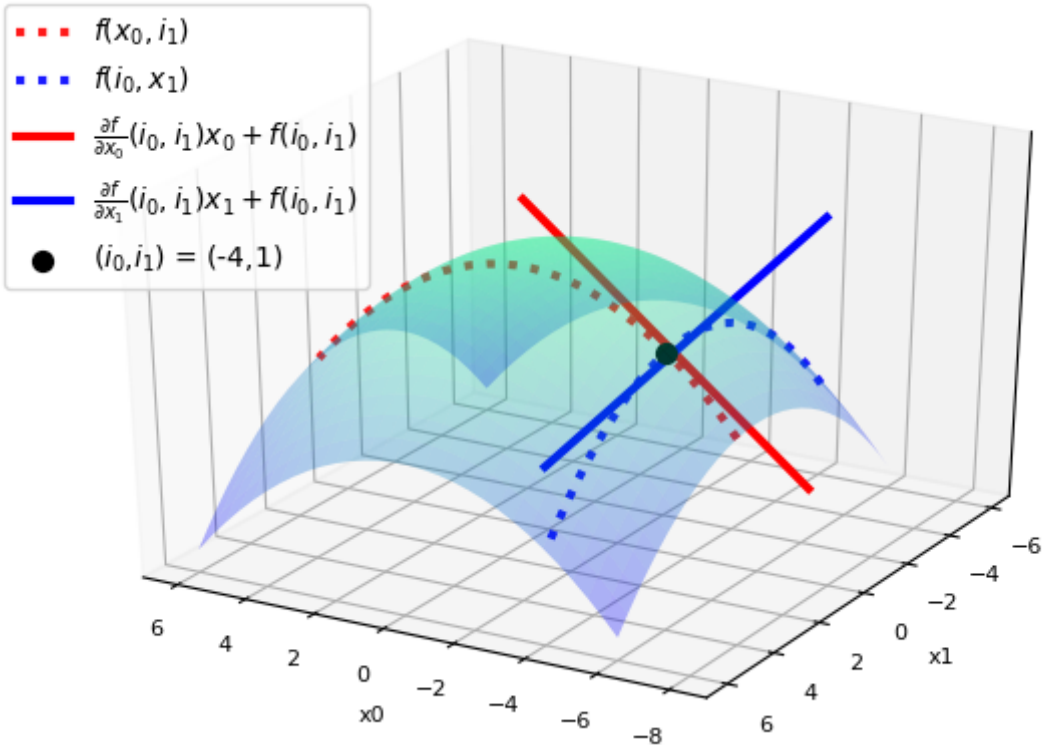
Basic operations

- Sums and products are denoted by capital Sigma and capital Pi:
$$\sum_{i=0}^{p} = x_0 + x_1 + \ldots + x_p \qquad \prod_{i=0}^{p} = x_0 \cdot x_1 \cdot \ldots \cdot x_p$$
- Operations on vectors are element-wise: e.g.
$\mathbf{x} + \mathbf{z} = [x_0 + z_0, x_1 + z_1, \ldots, x_p + z_p]$
- Dot product
$\mathbf{wx} = \mathbf{w} \cdot \mathbf{x} = \mathbf{w}^T\mathbf{x} = \sum_{i=0}^{p} w_i \cdot x_i = w_0 \cdot x_0 + w_1 \cdot x_1 + \ldots + w_p \cdot x_p$
- Matrix product $\mathbf{Wx} = \begin{bmatrix} \mathbf{w_0} \cdot \mathbf{x} \\ \ldots \\ \mathbf{w_p} \cdot \mathbf{x} \end{bmatrix}$
- A function $f(x) = y$ relates an input element x to an output y
  - It has a *local minimum* at $x = c$ if $f(x) \geq f(c)$ in interval $(c - \epsilon, c + \epsilon)$
  - It has a *global minimum* at $x = c$ if $f(x) \geq f(c)$ for any value for x
- A vector function consumes an input and produces a vector: $\mathbf{f}(\mathbf{x}) = \mathbf{y}$
- $\max_{x \in X} f(x)$ returns the highest value f(x) for any x
- $\operatorname{argmax}_{x \in X} f(x)$ returns the element x that maximizes f(x)

Gradients

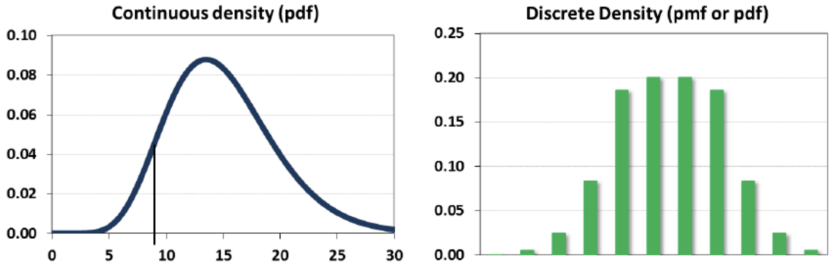
- A *derivative* f' of a function f describes how fast f grows or decreases
- The process of finding a derivative is called differentiation
  - Derivatives for basic functions are known
  - For non-basic functions we use the chain rule:
    $F(x) = f(g(x)) \rightarrow F'(x) = f'(g(x))g'(x)$
- A function is *differentiable* if it has a derivate in any point of it's domain
  - It's *continuously differentiable* if f' is itself a function
  - It's *smooth* if $f', f'', f''', \ldots$ all exist
- A *gradient* ∇f is the derivate of a function in multiple dimensions
  - It is a vector of partial derivatives: $\nabla f = \left[\frac{\partial f}{\partial x_0}, \frac{\partial f}{\partial x_1}, \ldots\right]$
  - E.g. $f = 2x_0 + 3x_1^2 - \sin(x_2) \rightarrow \nabla f = [2, 6x_1, -cos(x_2)]$

- Example: $f = -(x_0^2 + x_1^2)$
  - $\nabla f = \left[\frac{\partial f}{\partial x_0}, \frac{\partial f}{\partial x_1}\right] = [-2x_0, -2x_1]$
  - Evaluated at point (-4,1): $\nabla f(-4, 1) = [8, -2]$
    - These are the slopes at point (-4,1) in the direction of x_0 and x_1 respectively



Distributions and Probabilities

- The normal (Gaussian) distribution with mean μ and standard deviation σ is noted as $N(\mu, \sigma)$
- A random variable X can be continuous or discrete
- A probability distribution f_X of a continuous variable X: *probability density function* (pdf)
  - The *expectation* is given by $\mathbb{E}[X] = \int x f_X(x) dx$
- A probability distribution of a discrete variable: *probability mass function* (pmf)
  - The *expectation* (or mean) $\mu_X = \mathbb{E}[X] = \sum_{i=1}^{k} [x_i \cdot \boldsymbol{Pr}(X = x_i)]$



Linear models

Linear models make a prediction using a linear function of the input features X

$$f_{\mathbf{w}}(\mathbf{x}) = \sum_{i=1}^{p} w_i \cdot x_i + w_0$$

Learn w from X, given a loss function $\mathcal{L}$:

$$\underset{\mathbf{w}}{\operatorname{argmin}}\ \mathcal{L}(f_{\mathbf{w}}(X))$$

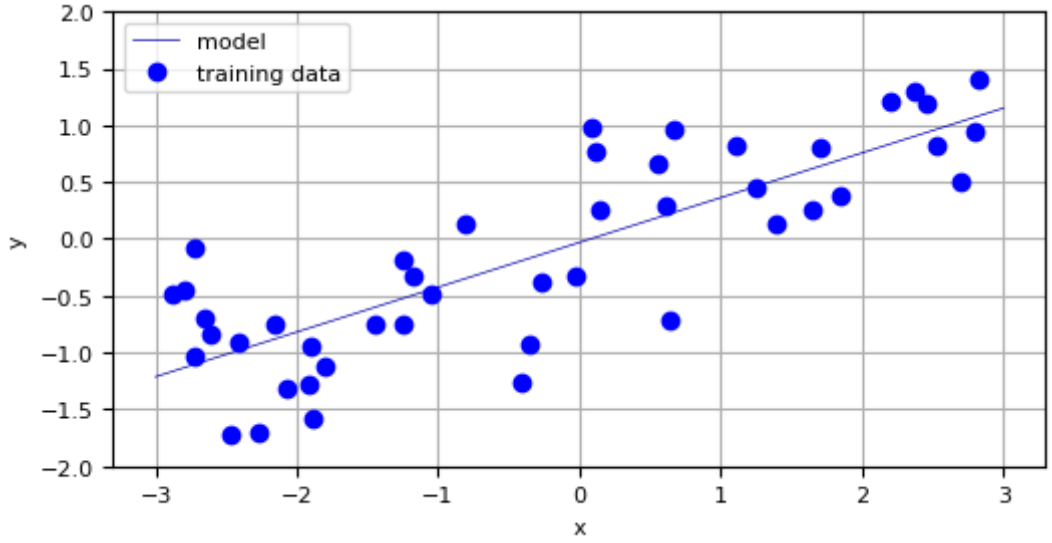
- Many algorithms with different $\mathcal{L}$: Least squares, Ridge, Lasso, Logistic Regression, Linear SVMs,...
- Can be very powerful (and fast), especially for large datasets with many features.
- Can be generalized to learn non-linear patterns: *Generalized Linear Models*
  - Features can be augmentented with polynomials of the original features
  - Features can be transformed according to a distribution (Poisson, Tweedie, Gamma,...)
  - Some linear models (e.g. SVMs) can be *kernelized* to learn non-linear functions

Linear models for regression

- Prediction formula for input features x:
  - w_1 ... w_p usually called *weights* or *coefficients* , w_0 the *bias* or *intercept*
  - Assumes that errors are $N(0, \sigma)$

$$\hat{y} = \mathbf{w}\mathbf{x} + w_0 = \sum_{i=1}^{p} w_i \cdot x_i + w_0 = w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_p \cdot x_p + w_0$$

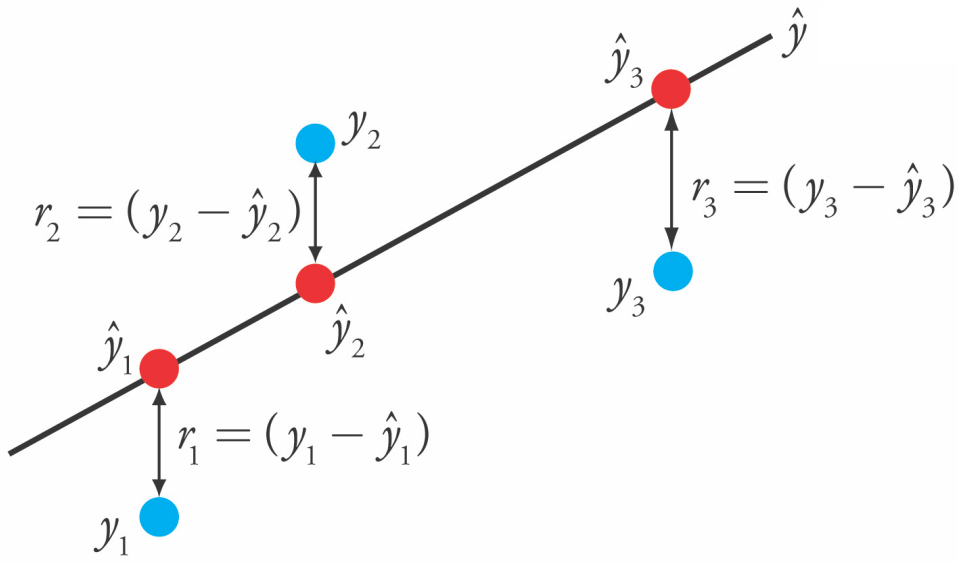
```
w_1: 0.393906  w_0: -0.031804
```



Linear Regression (aka Ordinary Least Squares)

- Loss function is the *sum of squared errors* (SSE) (or residuals) between predictions $\hat{y}_i$ (red) and the true regression targets y_i (blue) on the training set.

$$\mathcal{L}_{SSE} = \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 = \sum_{n=1}^{N} (y_n - (\mathbf{w}\mathbf{x_n} + w_0))^2$$



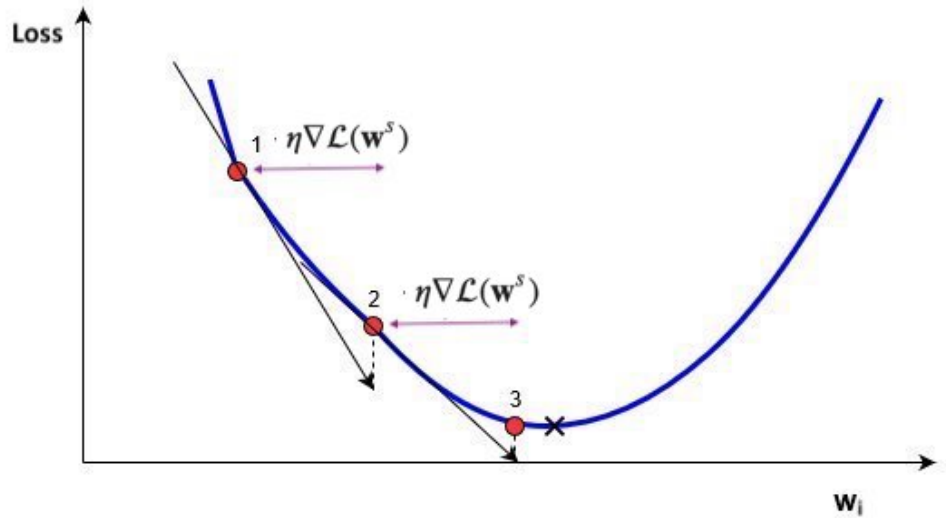
Solving ordinary least squares

- Convex optimization problem with unique closed-form solution:
$$w^* = (X^T X)^{-1} X^T Y$$
  - Add a column of 1's to the front of X to get w_0
  - Slow. Time complexity is quadratic in number of features: $\mathcal{O}(p^2 n)$
    - X has n rows, p features, hence $X^T X$ has dimensionality pxp
  - Only works if $n > p$
- *Gradient Descent*
  - Faster for large and/or high-dimensional datasets
  - When $X^T X$ cannot be computed or takes too long (p or n is too large)
- **Very easily overfits**.
  - coefficients w become very large (steep incline/decline)
  - small change in the input x results in a very different output y
  - No hyperparameters that control model complexity

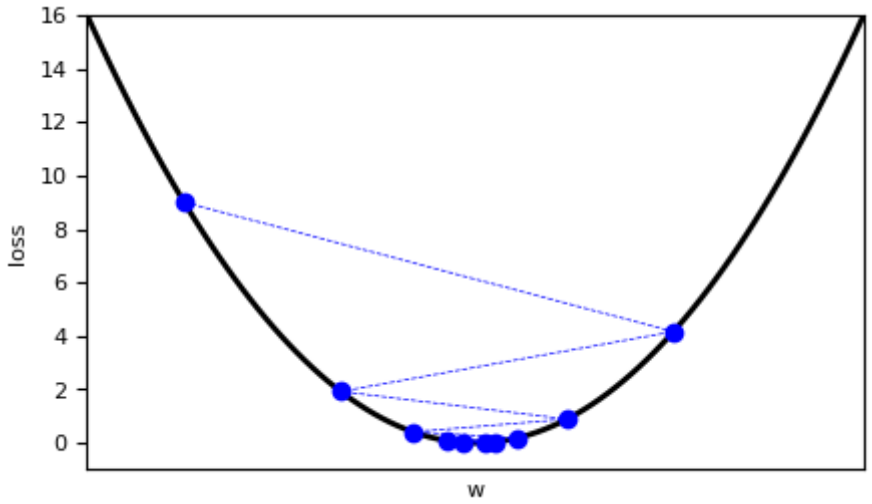
Gradient Descent

- Start with an initial, random set of weights: $\mathbf{w}^0$
- Given a differentiable loss function $\mathcal{L}$ (e.g. $\mathcal{L}_{SSE}$), compute $\nabla\mathcal{L}$
- For least squares: $\frac{\partial \mathcal{L}_{SSE}}{\partial w_i}(\mathbf{w}) = -2\sum_{n=1}^{N}(y_n - \hat{y}_n)x_{n,i}$
  - If feature $X_{:,i}$ is associated with big errors, the gradient wrt w_i will be large
- Update *all* weights slightly (by *step size* or *learning rate* η) in 'downhill' direction.
- Basic *update rule* (step s):

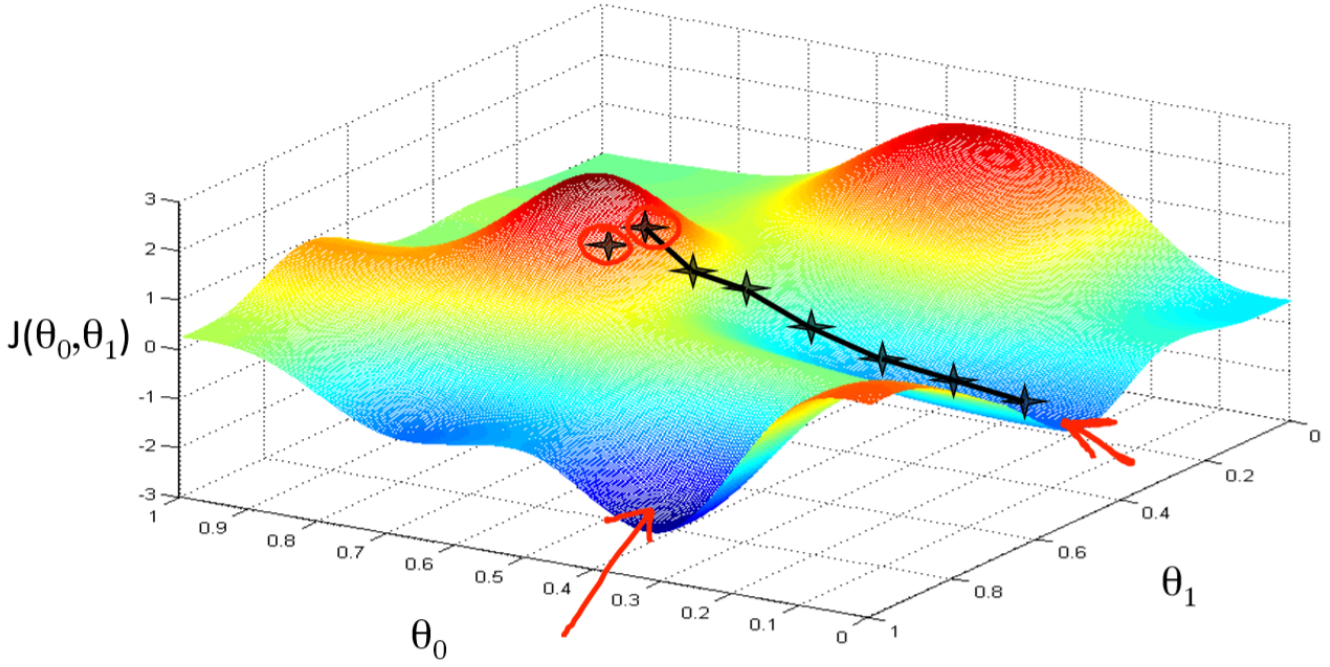
$$\mathbf{w}^{s+1} = \mathbf{w}^s - \eta\nabla\mathcal{L}(\mathbf{w}^s)$$



- Important hyperparameters
  - Learning rate
    - Too small: slow convergence. Too large: possible divergence
  - Maximum number of iterations
    - Too small: no convergence. Too large: wastes resources
  - Learning rate decay with decay rate k
    - E.g. exponential ($\eta^{s+1} = \eta^s e^{-ks}$), inverse-time ($\eta^{s+1} = \frac{\eta^0}{1+ks}$),...
  - Many more advanced ways to control learning rate (see later)
    - Adaptive techniques: depend on how much loss improved in previous step

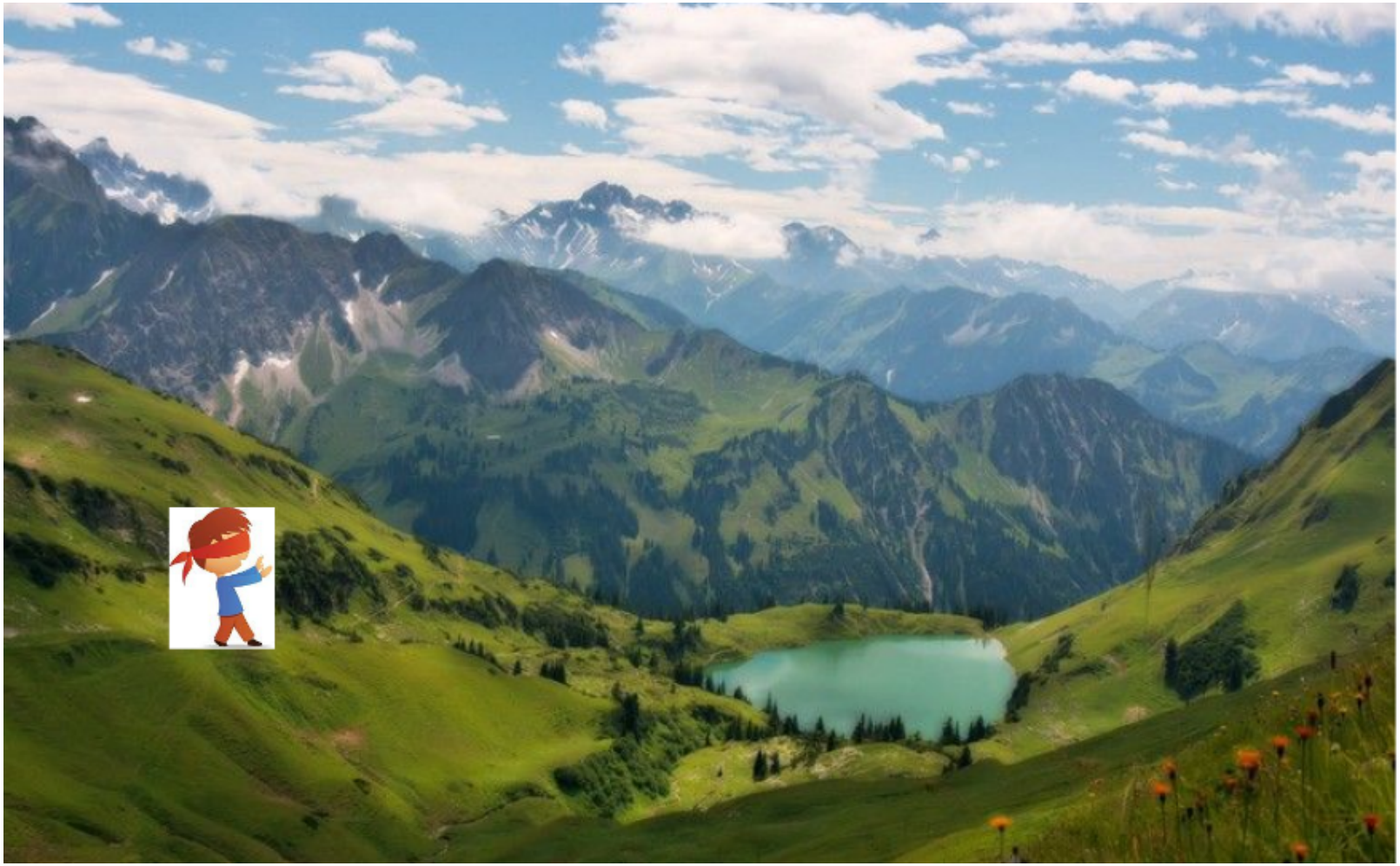


In two dimensions:



- You can get stuck in local minima (if the loss is not fully convex)
  - If you have many model parameters, this is less likely
  - You always find a way down in some direction
  - Models with many parameters typically find good local minima

- Intuition: walking downhill using only the slope you "feel" nearby

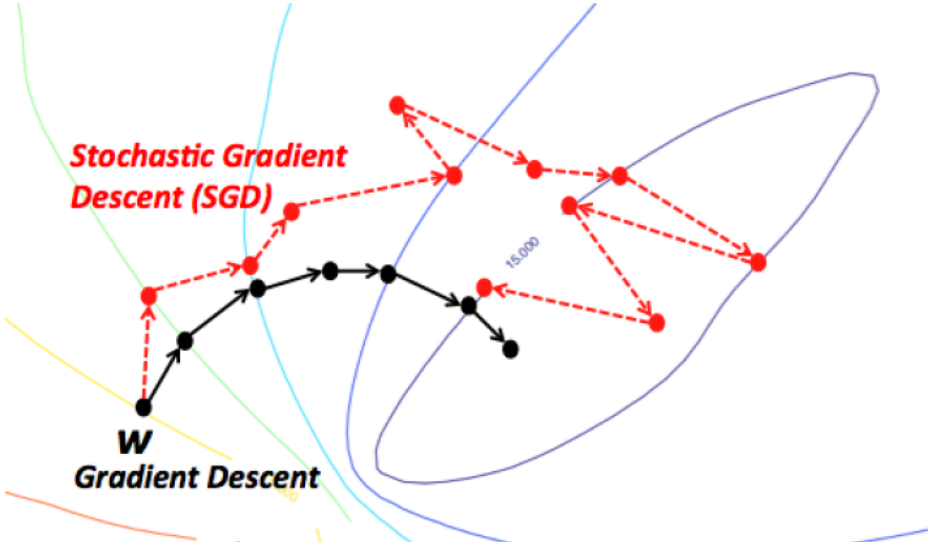


(Image by A. Karpathy)

Stochastic Gradient Descent (SGD)

- Compute gradients not on the entire dataset, but on a single data point i at a time
  - Gradient descent: $\mathbf{w}^{s+1} = \mathbf{w}^s - \eta \nabla \mathcal{L}(\mathbf{w}^s) = \mathbf{w}^s - \frac{\eta}{n} \sum_{i=0}^{n} \nabla \mathcal{L}_i(\mathbf{w}^s)$
  - Stochastic Gradient Descent: $\mathbf{w}^{s+1} = \mathbf{w}^s - \eta \nabla \mathcal{L}_i(\mathbf{w}^s)$
- Many smoother variants, e.g.
  - Minibatch SGD: compute gradient on batches of data: $\mathbf{w}^{s+1} = \mathbf{w}^s - \frac{\eta}{B} \sum_{i=0}^{B} \nabla \mathcal{L}_i(\mathbf{w}^s)$
  - Stochastic Average Gradient Descent (SAG, SAGA)
    - Incremental gradient: $\mathbf{w}^{s+1} = \mathbf{w}^s - \frac{\eta}{n} \sum_{i=0}^{n} v_i^s$ with

$$v_i^s = \begin{cases} \nabla \mathcal{L}_i(\mathbf{w}^s) & \text{random i} \\ v_i^{s-1} & \text{otherwise} \end{cases}$$



In practice

- Linear regression can be found in `sklearn.linear_model`. We'll evaluate it on the Boston Housing dataset.
  - `LinearRegression` uses closed form solution, `SGDRegressor` with `loss='squared_loss'` uses Stochastic Gradient Descent
  - Large coefficients signal overfitting
  - Test score is much lower than training score

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression().fit(X_train, y_train)
```

```
Weights (coefficients): [ -412.711   -52.243  -131.899   -12.004   -15.511
28.716    54.704
   -49.535    26.582    37.062   -11.828   -18.058   -19.525    12.203
  2980.781  1500.843   114.187   -16.97     40.961   -24.264    57.616
  1278.121 -2239.869   222.825    -2.182    42.996   -13.398   -19.389
    -2.575   -81.013     9.66      4.914    -0.812    -7.647    33.784
   -11.446    68.508   -17.375    42.813     1.14 ]
Bias (intercept): 30.934563673645666

Training set score (R^2): 0.95
Test set score (R^2): 0.61
```

Ridge regression

- Adds a penalty term to the least squares loss function:

$$\mathcal{L}_{Ridge} = \sum_{n=1}^{N}(y_n - (\mathbf{w}\mathbf{x_n} + w_0))^2 + \alpha \sum_{i=1}^{p} w_i^2$$

- Model is penalized if it uses large coefficients (w)
  - Each feature should have as little effect on the outcome as possible
- Regularization: explicitly restrict a model to avoid overfitting.
  - Called L2 regularization because it uses the L2 norm: $\sum w_i^2$
- The strength of the regularization can be controlled with the α hyperparameter.
  - Increasing α causes more regularization (or shrinkage). Default is 1.0.
- Still convex. Can be optimized in different ways:
  - Closed form solution (a.k.a. Cholesky): $w^* = (X^T X + \alpha I)^{-1} X^T Y$
  - Gradient descent and variants, e.g. Stochastic Average Gradient (SAG,SAGA)
    - Conjugate gradient (CG): each new gradient is influenced by previous ones
  - Use Cholesky for smaller datasets, Gradient descent for larger ones

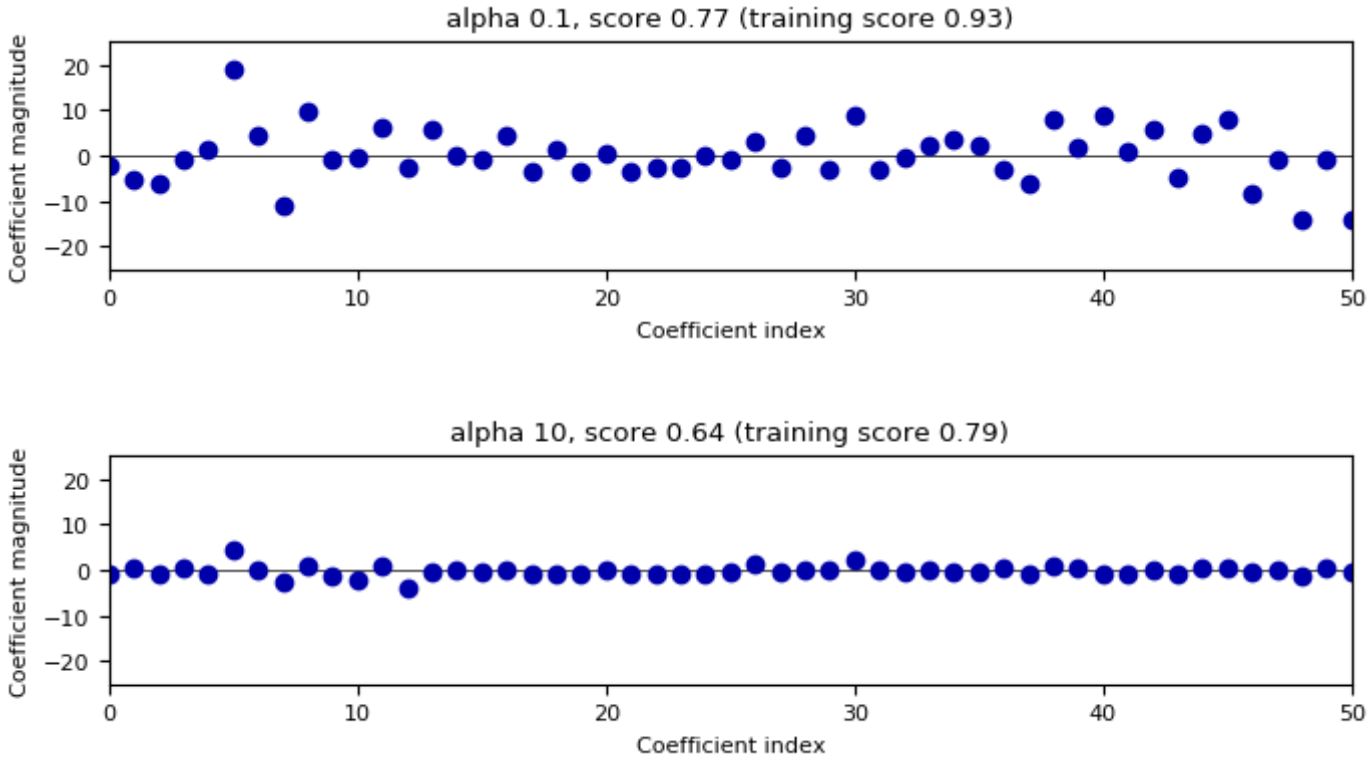
In practice

```
from sklearn.linear_model import Ridge
lr = Ridge().fit(X_train, y_train)
```

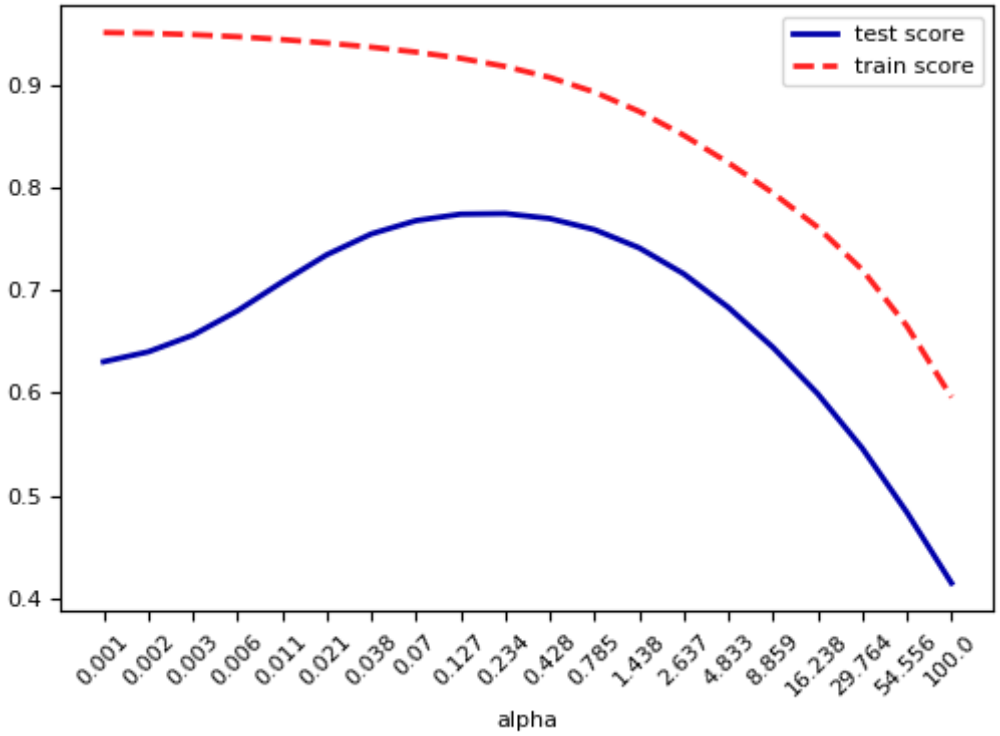
```
Weights (coefficients): [-1.414 -1.557 -1.465 -0.127 -0.079  8.332  0.255 -4.9
41  3.899 -1.059
 -1.584  1.051 -4.012  0.334  0.004 -0.849  0.745 -1.431 -1.63  -1.405
 -0.045 -1.746 -1.467 -1.332 -1.692 -0.506  2.622 -2.092  0.195 -0.275
  5.113 -1.671 -0.098  0.634 -0.61   0.04  -1.277 -2.913  3.395  0.792]
Bias (intercept): 21.390525958609967
Training set score: 0.89
Test set score: 0.75
```

Test set score is higher and training set score lower: less overfitting!

- We can plot the weight values for differents levels of regularization to explore the effect of α.
- Increasing regularization decreases the values of the coefficients, but never to 0.

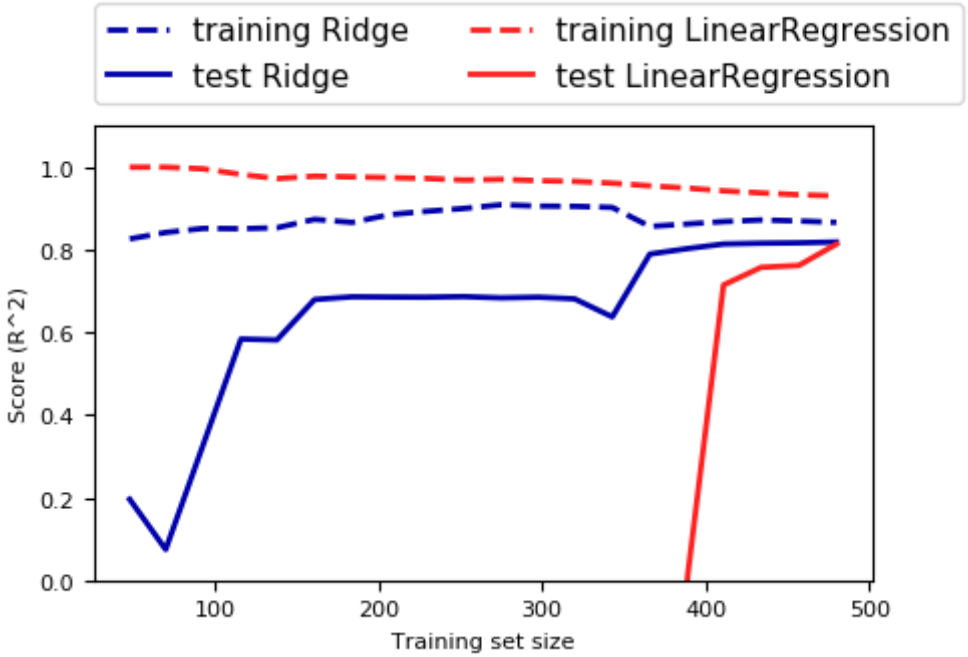


- When we plot the train and test scores for every α value, we see a sweet spot around $\alpha = 0.2$
  - Models with smaller α are overfitting
  - Models with larger α are underfitting



Other ways to reduce overfitting

- Add more training data: with enough training data, regularization becomes less important
  - Ridge and ordinary least squares will have the same performance
- Use fewer features: remove unimportant ones or find a low-dimensional embedding (e.g. PCA)
  - Fewer coefficients to learn, reduces the flexibility of the model
- Scaling the data typically helps (and changes the optimal α value)



Lasso (Least Absolute Shrinkage and Selection Operator)

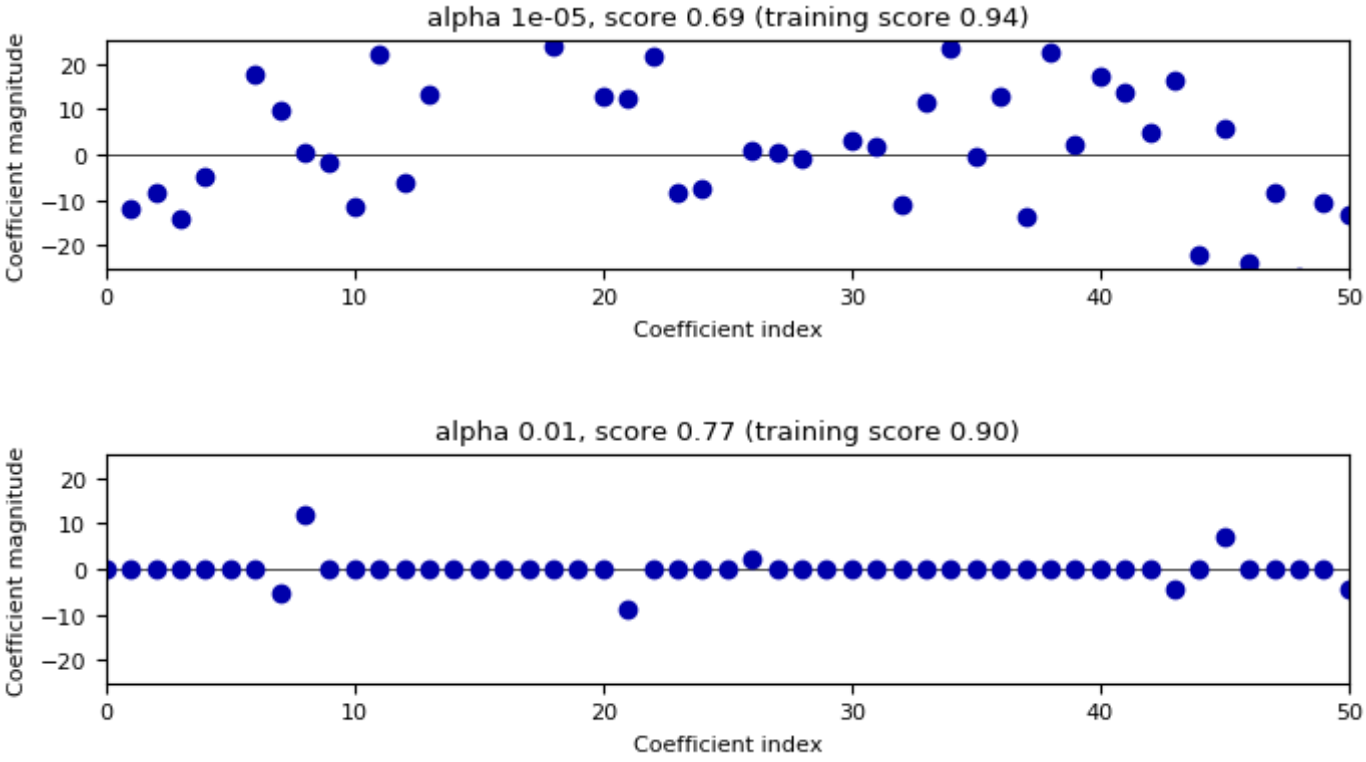
- Adds a different penalty term to the least squares sum:

$$\mathcal{L}_{Lasso} = \sum_{n=1}^{N}(y_n - (\mathbf{w}\mathbf{x_n} + w_0))^2 + \alpha \sum_{i=1}^{p} |w_i|$$

- Called L1 regularization because it uses the L1 norm
  - Will cause many weights to be exactly 0
- Same parameter α to control the strength of regularization.
  - Will again have a 'sweet spot' depending on the data
- No closed-form solution
- Convex, but no longer strictly convex, and not differentiable
  - Weights can be optimized using *coordinate descent*

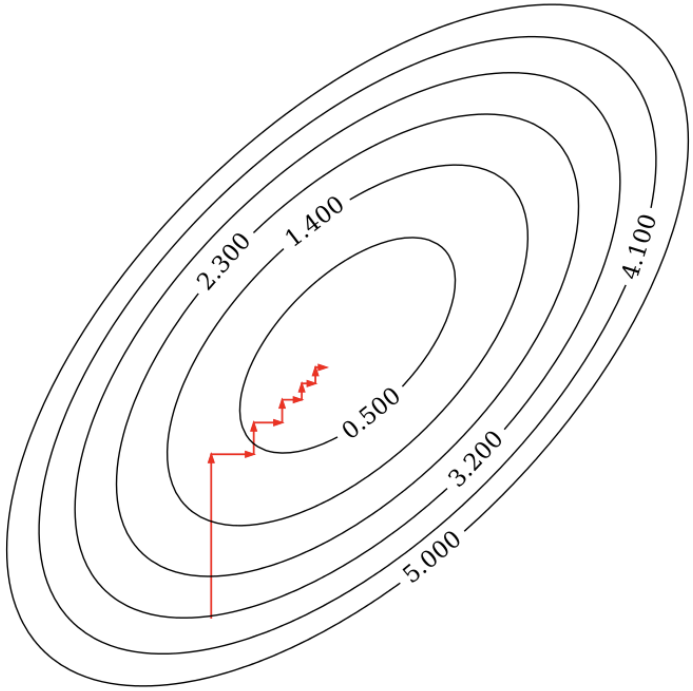
Analyze what happens to the weights:

- L1 prefers coefficients to be exactly zero (sparse models)
- Some features are ignored entirely: automatic feature selection
- How can we explain this?



Coordinate descent

- Alternative for gradient descent, supports non-differentiable convex loss functions (e.g. $\mathcal{L}_{Lasso}$)
- In every iteration, optimize a single coordinate w_i (find minimum in direction of x_i)
  - Continue with another coordinate, using a selection rule (e.g. round robin)
- Faster iterations. No need to choose a step size (learning rate).
- May converge more slowly. Can't be parallellized.



Coordinate descent with Lasso

- Remember that $\mathcal{L}_{Lasso} = \mathcal{L}_{SSE} + \alpha \sum_{i=1}^{p} |w_i|$
- For one w_i: $\mathcal{L}_{Lasso}(w_i) = \mathcal{L}_{SSE}(w_i) + \alpha|w_i|$

- The L1 term is not differentiable but convex: we can compute the *subgradient* (https://towardsdatascience.com/unboxing-lasso-regularization-with-proximal-gradient-method-ista-iterative-soft-thresholding-b0797f05f8ea)
  - Unique at points where $\mathcal{L}$ is differentiable, a range of all possible slopes [a,b] where it is not
  - For $|w_i|$, the subgradient $\partial_{w_i}|w_i| = \begin{cases} -1 & w_i < 0 \\ [-1, 1] & w_i = 0 \\ 1 & w_i > 0 \end{cases}$
  - Subdifferential $\partial(f + g) = \partial f + \partial g$ if f and g are both convex

- To find the optimum for Lasso w_i^*, solve

$$\begin{aligned} \partial_{w_i}\mathcal{L}_{Lasso}(w_i) &= \partial_{w_i}\mathcal{L}_{SSE}(w_i) + \partial_{w_i}\alpha|w_i| \\ 0 &= (w_i - \rho_i) + \alpha \cdot \partial_{w_i}|w_i| \\ w_i &= \rho_i - \alpha \cdot \partial_{w_i}|w_i| \end{aligned}$$

  - In which ρ_i is the solution for $\mathcal{L}_{SSE}(w_i)$

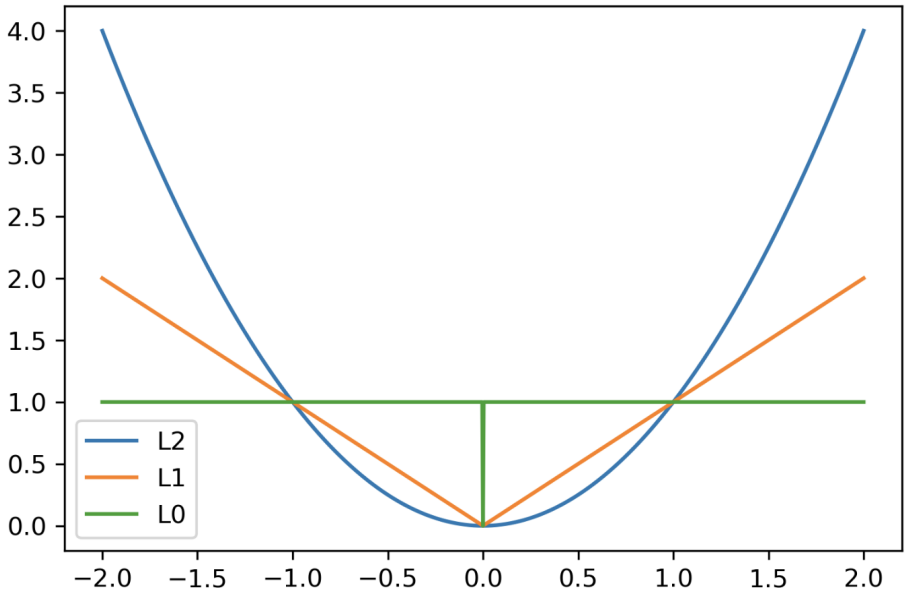
- We found: $w_i = \rho_i - \alpha \cdot \partial_{w_i} |w_i|$
- Lasso solution has the form of a *soft thresholding function* S

$$w_i^* = S(\rho_i, \alpha) = \begin{cases} \rho_i + \alpha, & \rho_i < -\alpha \\ 0, & -\alpha < \rho_i < \alpha \\ \rho_i - \alpha, & \rho_i > \alpha \end{cases}$$

  - Small weights become 0: sparseness!
  - If the data is not normalized, $w_i^* = \frac{1}{z_i} S(\rho_i, \alpha)$ with z_i a normalizing constant
- Ridge solution: $w_i = \rho_i - \alpha \cdot \partial_{w_i} w_i^2 = \rho_i - 2\alpha \cdot w_i$, thus $w_i^* = \frac{\rho_i}{1+2\alpha}$

Interpreting L1 and L2 loss

- L1 and L2 in function of the weights



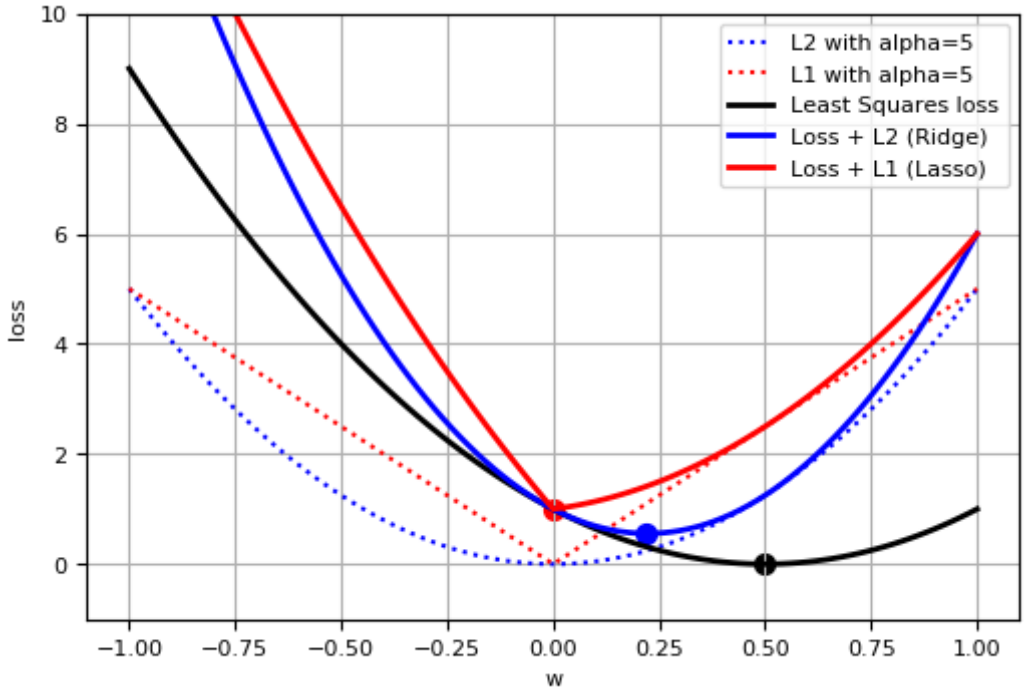
$$\ell_2(w) = \sqrt{\sum_i w_i^2}$$

$$\ell_1(w) = \sum_i |w_i|$$

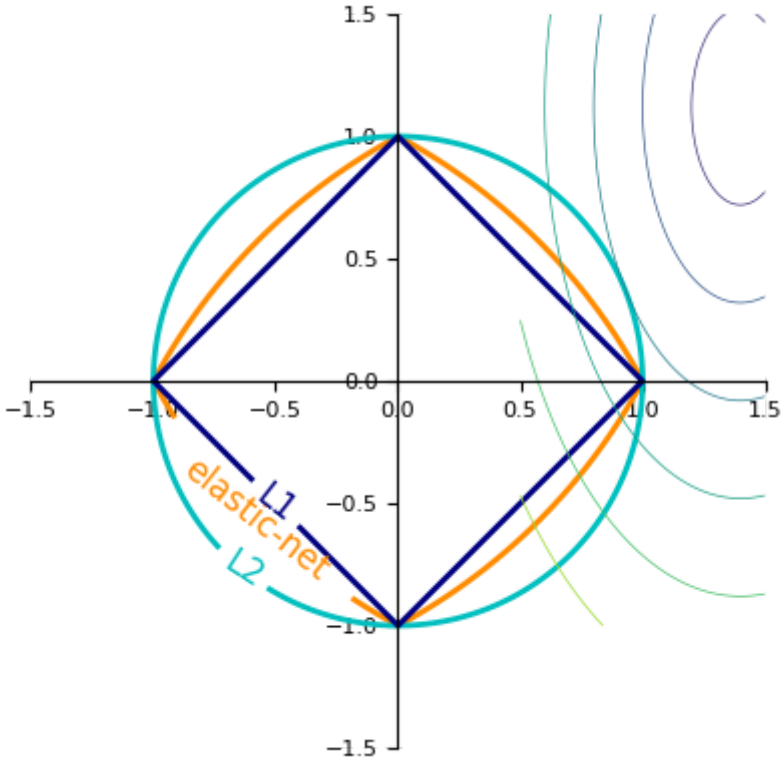
$$\ell_0(w) = \sum_i 1_{w_i!=0}$$

Least Squares Loss + L1 or L2

- Lasso is not differentiable at point 0
- For any minimum of least squares, L2 will be smaller, and L1 is more likely be 0



- In 2D (for 2 model weights w_1 and w_2)
  - The least squared loss is a 2D convex function in this space
  - For illustration, assume that L1 loss = L2 loss = 1
    - L1 loss ($\Sigma|w_i|$): every $\{w_1, w_2\}$ falls on the diamond
    - L2 loss (Σw_i^2): every $\{w_1, w_2\}$ falls on the circle
  - For L1, the loss is minimized if w_1 or w_2 is 0 (rarely so for L2)



Elastic-Net

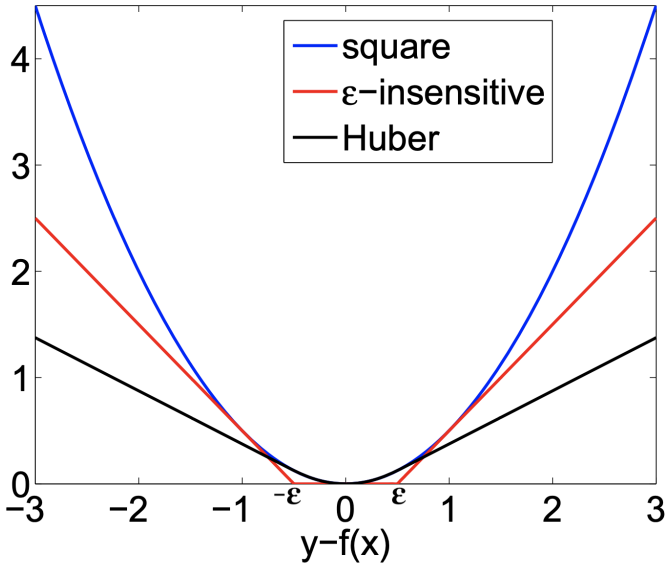
- Adds both L1 and L2 regularization:

$$\mathcal{L}_{Elastic} = \sum_{n=1}^{N}(y_n - (\mathbf{w}\mathbf{x_n} + w_0))^2 + \alpha\rho \sum_{i=1}^{p} |w_i| + \alpha(1-\rho) \sum_{i=1}^{p} w_i^2$$

- ρ is the L1 ratio
  - With $\rho = 1$, $\mathcal{L}_{Elastic} = \mathcal{L}_{Lasso}$
  - With $\rho = 0$, $\mathcal{L}_{Elastic} = \mathcal{L}_{Ridge}$
  - $0 < \rho < 1$ sets a trade-off between L1 and L2.
- Allows learning sparse models (like Lasso) while maintaining L2 regularization benefits
  - E.g. if 2 features are correlated, Lasso likely picks one randomly, Elastic-Net keeps both
- Weights can be optimized using coordinate descent (similar to Lasso)

Other loss functions for regression

- Huber loss: switches from squared loss to linear loss past a value ϵ
  - More robust against outliers
- Epsilon insensitive: ignores errors smaller than ϵ, and linear past that
  - Aims to fit function so that residuals are at most ϵ
  - Also known as Support Vector Regression (`SVR` in sklearn)
- Squared Epsilon insensitive: ignores errors smaller than ϵ, and squared past that
- These can all be solved with stochastic gradient descent
  - `SGDRegressor` in sklearn

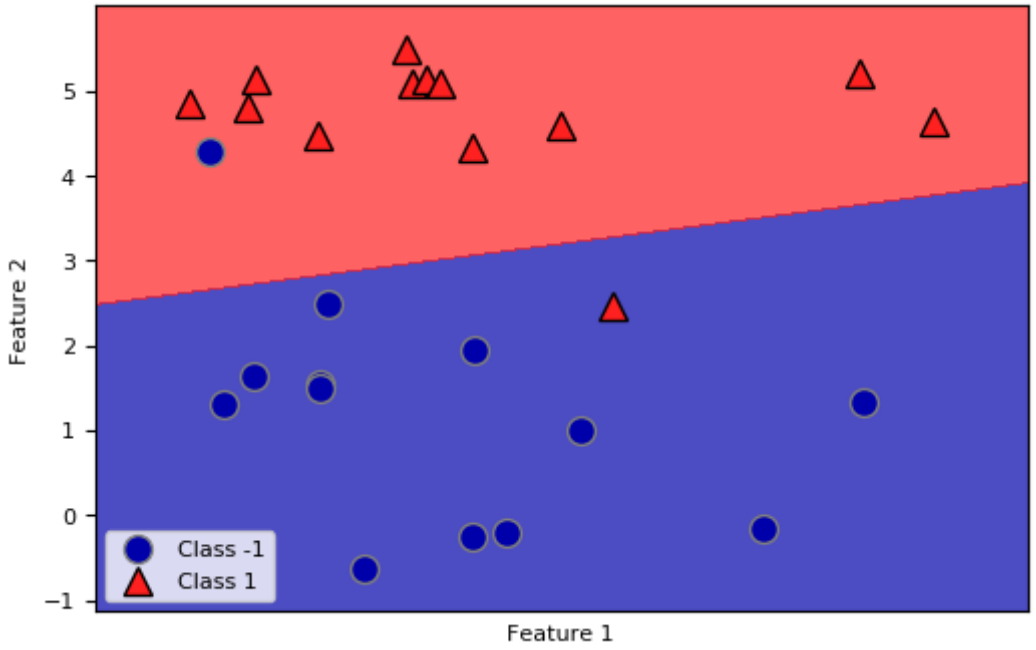


Linear models for Classification

Aims to find a hyperplane that separates the examples of each class.
For binary classification (2 classes), we aim to fit the following function:

$$\hat{y} = w_1 * x_1 + w_2 * x_2 + \ldots + w_p * x_p + w_0 > 0$$

When $\hat{y} < 0$, predict class -1, otherwise predict class +1



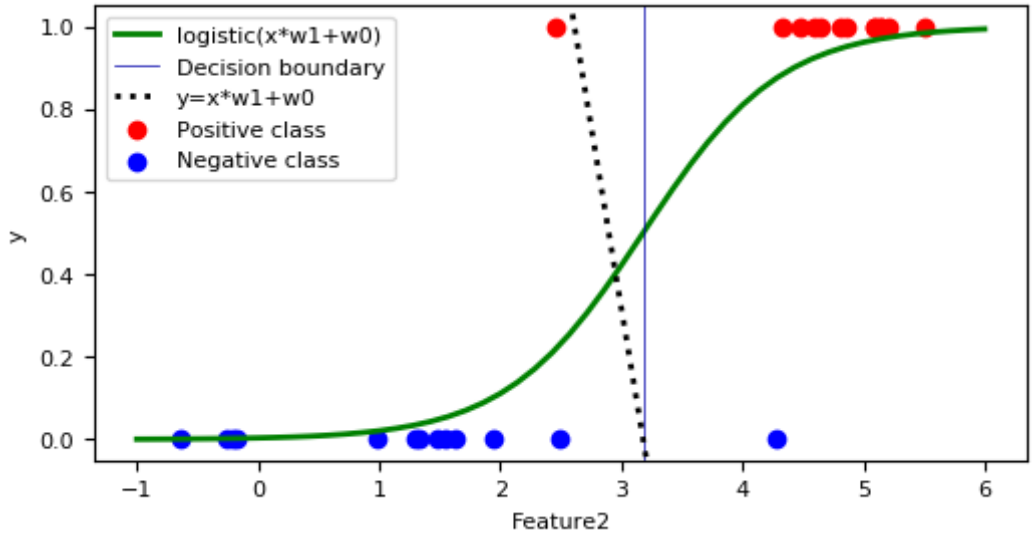
- There are many algorithms for linear classification, differing in loss function, regularization techniques, and optimization method
- Most common techniques:
  - Convert target classes {neg,pos} to {0,1} and treat as a regression task
    - Logistic regression (Log loss)
    - Ridge Classification (Least Squares + L2 loss)
  - Find hyperplane that maximizes the margin between classes
    - Linear Support Vector Machines (Hinge loss)
  - Neural networks without activation functions
    - Perceptron (Perceptron loss)
  - SGDClassifier: can act like any of these by choosing loss function
    - Hinge, Log, Modified_huber, Squared_hinge, Perceptron

Logistic regression

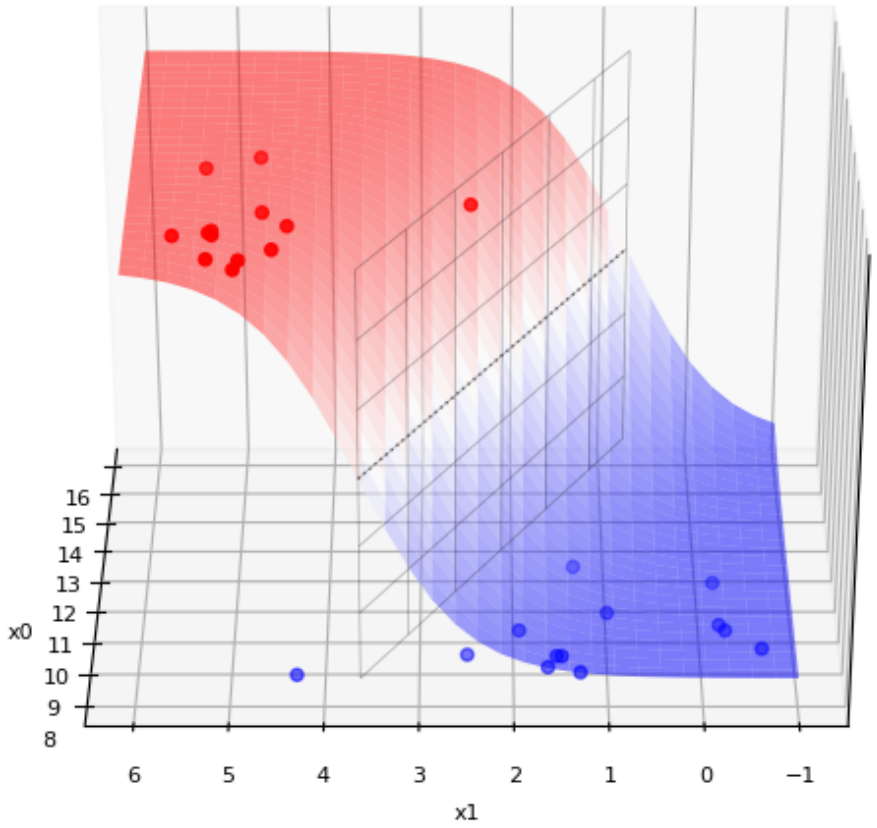
- Aims to predict the *probability* that a point belongs to the positive class
- Converts target values {negative (blue), positive (red)} to {0,1}
- Fits a *logistic* (or *sigmoid* or *S* curve) function through these points
  - Maps (-Inf,Inf) to a probability [0,1]

$$\hat{y} = \text{logistic}(f_\theta(\mathbf{x})) = \frac{1}{1 + e^{-f_\theta(\mathbf{x})}}$$

- E.g. in 1D: $\text{logistic}(x_1 w_1 + w_0) = \frac{1}{1+e^{-x_1 w_1 - w_0}}$



- Fitted solution to our 2D example:
  - To get a binary prediction, choose a probability threshold (e.g. 0.5)

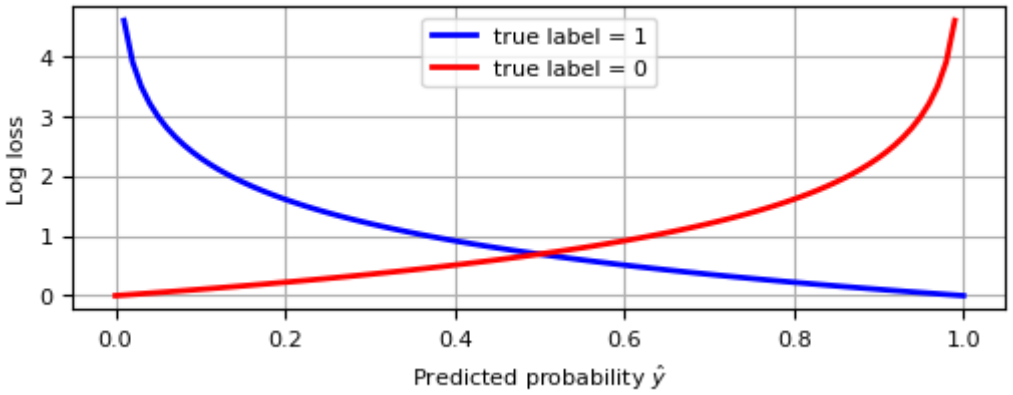


Loss function: Cross-entropy

- Models that return class probabilities can use *cross-entropy loss*

$$\mathcal{L}_{log}(\mathbf{w}) = \sum_{n=1}^{N} H(p_n, q_n) = -\sum_{n=1}^{N}\sum_{c=1}^{C} p_{n,c} log(q_{n,c})$$

  - Also known as log loss, logistic loss, or maximum likelihood
  - Based on true probabilities p (0 or 1) and predicted probabilities q over N instances and C classes
    - Binary case (C=2): $\mathcal{L}_{log}(\mathbf{w}) = -\sum_{n=1}^{N} \left[y_n log(\hat{y_n}) + (1 - y_n) log(1 - \hat{y_n}) \right]$
  - Penalty (or surprise) grows exponentially as difference between p and q increases
  - Often used together with L2 (or L1) loss: $\mathcal{L}_{log}{}'(\mathbf{w}) = \mathcal{L}_{log}(\mathbf{w}) + \alpha \sum_i w_i^2$



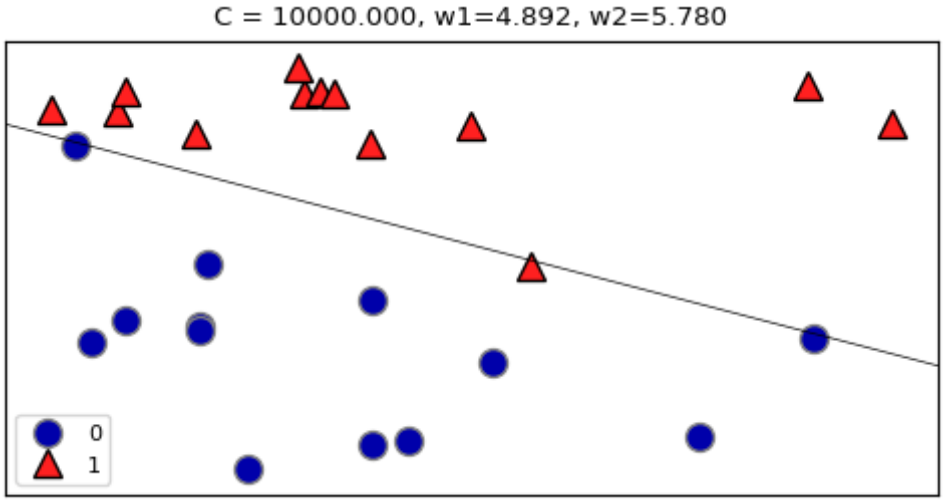
Optimization methods (solvers) for cross-entropy loss

- Gradient descent (only supports L2 regularization)
  - Log loss is differentiable, so we can use (stochastic) gradient descent
  - Variants thereof, e.g. Stochastic Average Gradient (SAG, SAGA)
- Coordinate descent (supports both L1 and L2 regularization)
  - Faster iteration, but may converge more slowly, has issues with saddlepoints
  - Called `liblinear` in sklearn. Can't run in parallel.
- Newton-Rhapson or Newton Conjugate Gradient (only L2):
  - Uses the Hessian $H = \left[\frac{\partial^2 \mathcal{L}}{\partial x_i \partial x_j}\right]$: $\mathbf{w}^{s+1} = \mathbf{w}^s - \eta H^{-1}(\mathbf{w}^s)\nabla\mathcal{L}(\mathbf{w}^s)$
  - Slow for large datasets. Works well if solution space is (near) convex
- Quasi-Newton methods (only L2)
  - Approximate, faster to compute
  - E.g. Limited-memory Broyden–Fletcher–Goldfarb–Shanno (`lbfgs`)
    - Default in sklearn for Logistic Regression
- Some hints on choosing solvers (https://towardsdatascience.com/dont-sweat-the-solver-stuff-aea7cddc3451)
  - Data scaling helps convergence, minimizes differences between solvers

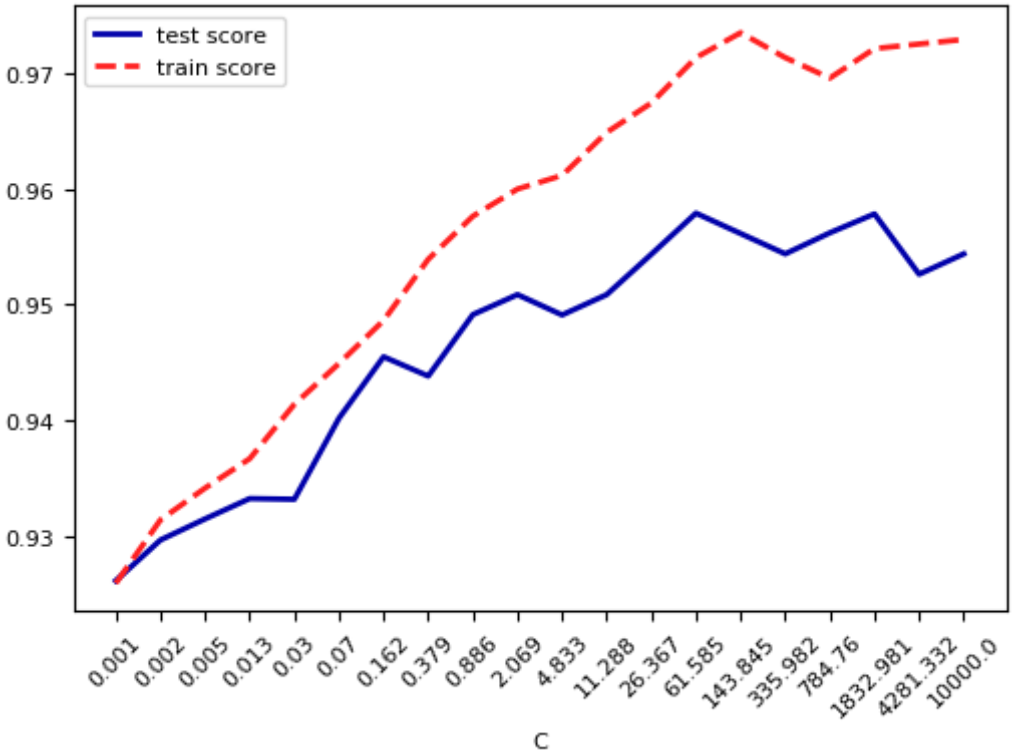
In practice

- Logistic regression can also be found in `sklearn.linear_model`.
  - `C` hyperparameter is the *inverse* regularization strength: $C = \alpha^{-1}$
  - `penalty`: type of regularization: L1, L2 (default), Elastic-Net, or None
  - `solver`: newton-cg, lbfgs (default), liblinear, sag, saga
- Increasing C: less regularization, tries to overfit individual points

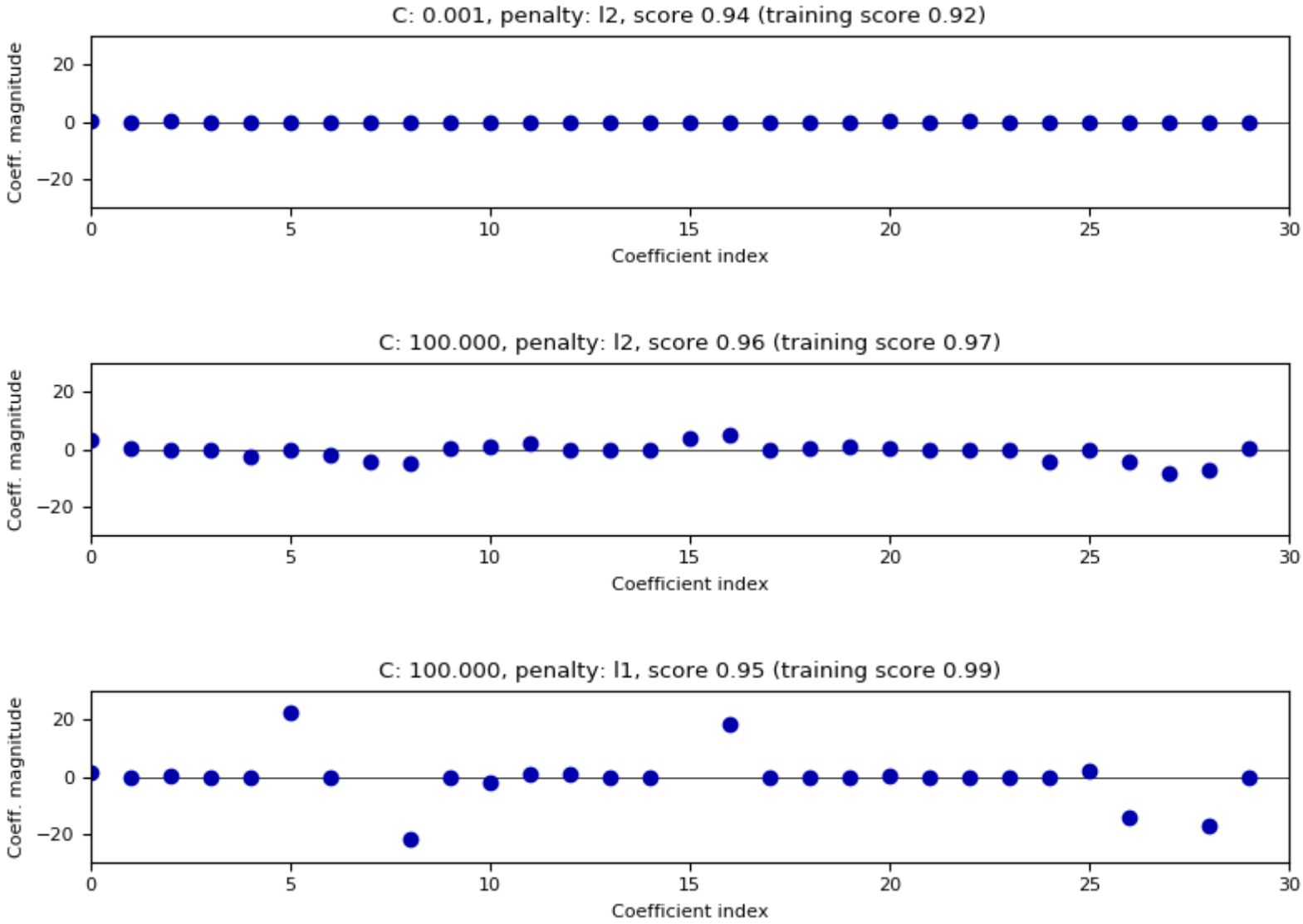
```
from sklearn.linear_model import LogisticRegression
lr = LogisticRegression(C=1).fit(X_train, y_train)
```



- Analyze behavior on the breast cancer dataset
  - Underfitting if C is too small, some overfitting if C is too large
  - We use cross-validation because the dataset is small



- Again, choose between L1 or L2 regularization (or elastic-net)
- Small C overfits, L1 leads to sparse models



Ridge Classification

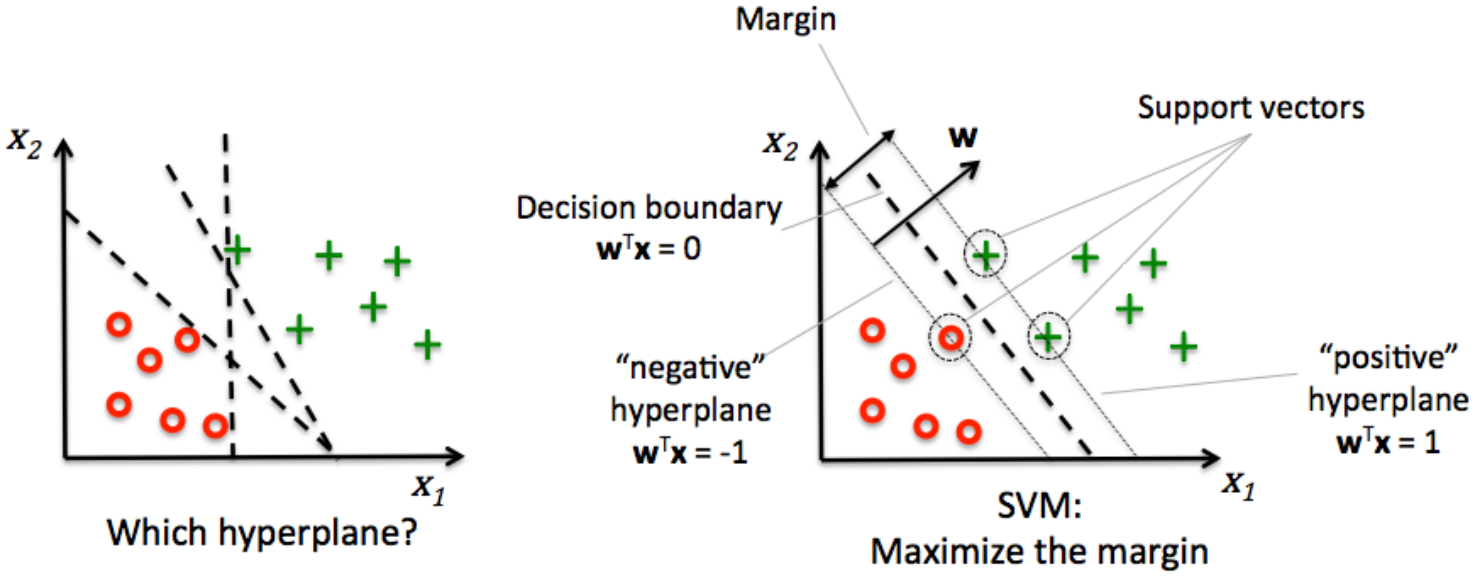
- Instead of log loss, we can also use ridge loss:

$$\mathcal{L}_{Ridge} = \sum_{n=1}^{N}(y_n - (\mathbf{wx_n} + w_0))^2 + \alpha \sum_{i=1}^{p} w_i^2$$

- In this case, target values {negative, positive} are converted to {-1,1}
- Can be solved similarly to Ridge regression:
  - Closed form solution (a.k.a. Cholesky)
  - Gradient descent and variants
    - E.g. Conjugate Gradient (CG) or Stochastic Average Gradient (SAG,SAGA)
  - Use Cholesky for smaller datasets, Gradient descent for larger ones

Support vector machines

- Decision boundaries close to training points may generalize badly
  - Very similar (nearby) test point are classified as the other class
- Choose a boundary that is as far away from training points as possible
- The **support vectors** are the training samples closest to the hyperplane
- The **margin** is the distance between the separating hyperplane and the *support vectors*
- Hence, our objective is to *maximize the margin*

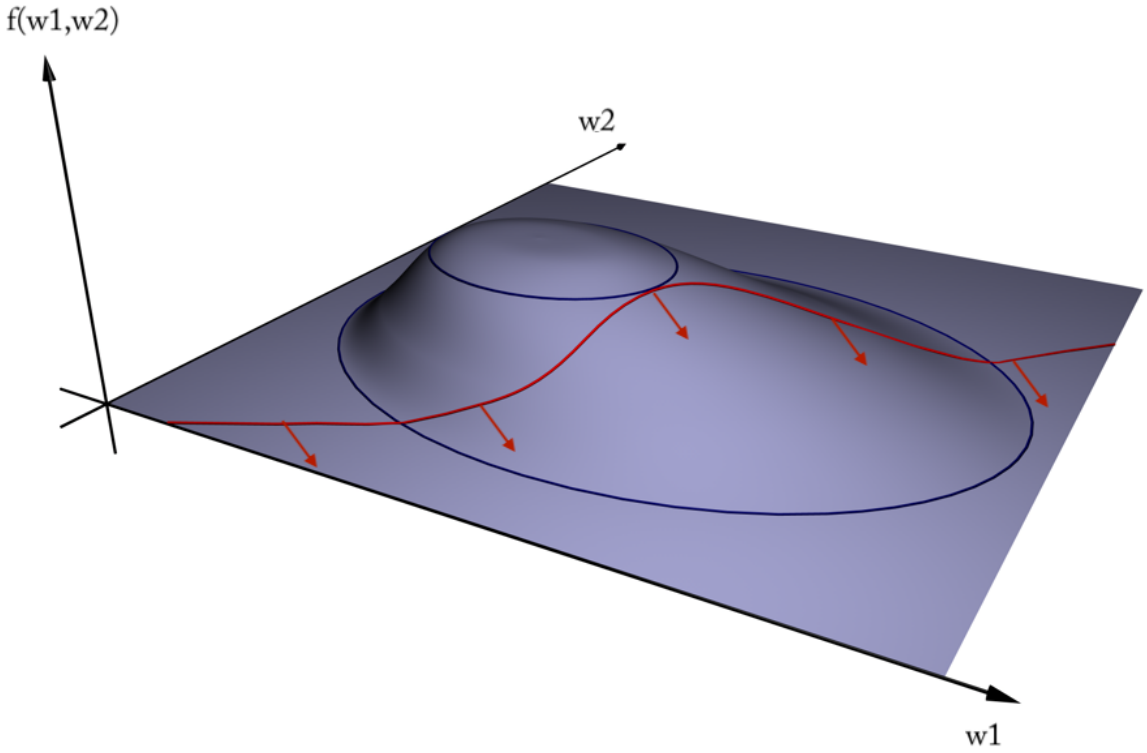


Solving SVMs with Lagrange Multipliers

- Imagine a hyperplane (green) $y = \sum_1^p \mathbf{w}_i * \mathbf{x}_i + w_0$ that has slope $\mathbf{w}$, value '+1' for the positive (red) support vectors, and '-1' for the negative (blue) ones
  - Margin between the boundary and support vectors is $\frac{y - w_0}{||\mathbf{w}||}$, with $||\mathbf{w}|| = \sum_i^p w_i^2$
  - We want to find the weights that maximize $\frac{1}{||\mathbf{w}||}$. We can also do that by maximizing $\frac{1}{||\mathbf{w}||^2}$

Geometric interpretation

- We want to maximize $f = \frac{1}{||w||^2}$ (blue contours)
- The hyperplane (red) must be > 1 for all positive examples: $g(\mathbf{w}) = \mathbf{wx_i} + w_0 > 1 \quad \forall i, y(i) = 1$
- Find the weights $\mathbf{w}$ that satify g but maximize f



Solution

- A quadratic loss function with linear constraints can be solved with *Lagrangian multipliers*
- This works by assigning a weight a_i (called a dual coefficient) to every data point x_i
  - They reflect how much individual points influence the weights $\mathbf{w}$
  - The points with non-zero a_i are the *support vectors*
- Next, solve the following **Primal** objective:
  - $y_i = \pm 1$ is the correct class for example x_i

$$\mathcal{L}_{Primal} = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} a_i y_i(\mathbf{w}\mathbf{x_i} + w_0) + \sum_{i=1}^{n} a_i$$

so that

$$\mathbf{w} = \sum_{i=1}^{n} a_i y_i \mathbf{x_i}$$

$$a_i \geq 0 \quad \text{and} \quad \sum_{i=1}^{l} a_i y_i = 0$$

- It has a **Dual** formulation as well (See 'Elements of Statistical Learning' for the derivation):

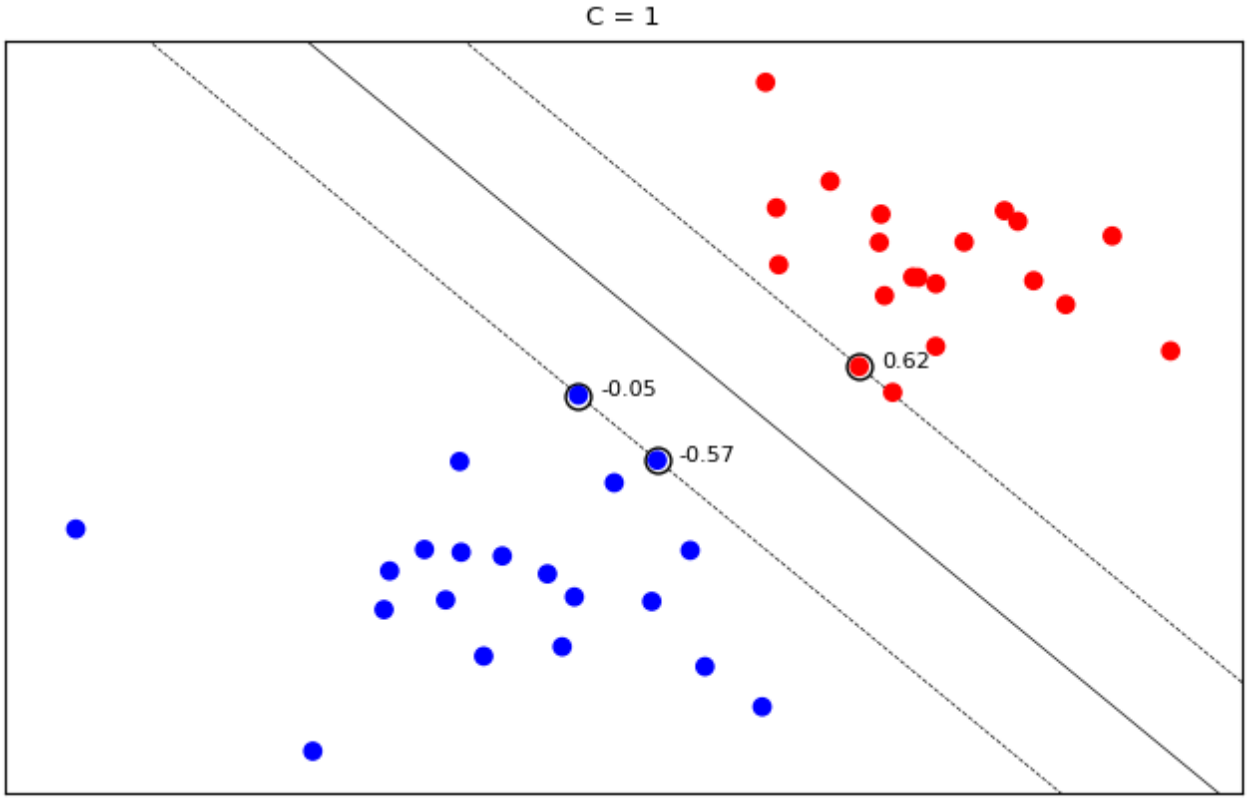
$$\mathcal{L}_{Dual} = \sum_{i=1}^{l} a_i - \frac{1}{2} \sum_{i,j=1}^{l} a_i a_j y_i y_j (\mathbf{x_i} \mathbf{x_j})$$

so that

$$a_i \geq 0 \quad \text{and} \quad \sum_{i=1}^{l} a_i y_i = 0$$

- Computes the dual coefficients directly. A number l of these are non-zero (sparseness).
  - Dot product $\mathbf{x_i} \mathbf{x_j}$ can be interpreted as the closeness between points $\mathbf{x_i}$ and $\mathbf{x_j}$
  - $\mathcal{L}_{Dual}$ increases if nearby support vectors $\mathbf{x_i}$ with high weights a_i have different class y_i
  - $\mathcal{L}_{Dual}$ also increases with the number of support vectors l and their weights a_i
- Can be solved with quadratic programming, e.g. Sequential Minimal Optimization (SMO)

Example result. The circled samples are support vectors, together with their coefficients.



Making predictions

- a_i will be *0* if the training point lies on the right side of the decision boundary and outside the margin
- The training samples for which a_i is not 0 are the *support vectors*

- Hence, the SVM model is completely defined by the support vectors and their dual coefficients (weights)

- Knowing the dual coefficients a_i, we can find the weights w for the maximal margin separating hyperplane:

$$\mathbf{w} = \sum_{i=1}^{l} a_i \, y_i \, \mathbf{x_i}$$

- Hence, we can classify a new sample $\mathbf{u}$ by looking at the sign of $\mathbf{wu} + w_0$

SVMs and kNN

- Remember, we will classify a new point $\mathbf{u}$ by looking at the sign of:

$$f(x) = \mathbf{wu} + w_0 = \sum_{i=1}^{l} a_i y_i \mathbf{x_i u} + w_0$$

- *Weighted k-nearest neighbor* is a generalization of the k-nearest neighbor classifier. It classifies points by evaluating:

$$f(x) = \sum_{i=1}^{k} a_i y_i dist(x_i, u)^{-1}$$

- Hence: SVM's predict much the same way as k-NN, only:
  - They only consider the truly important points (the support vectors): *much* faster
    - The number of neighbors is the number of support vectors
  - The distance function is an *inner product of the inputs*

Regularized (soft margin) SVMs

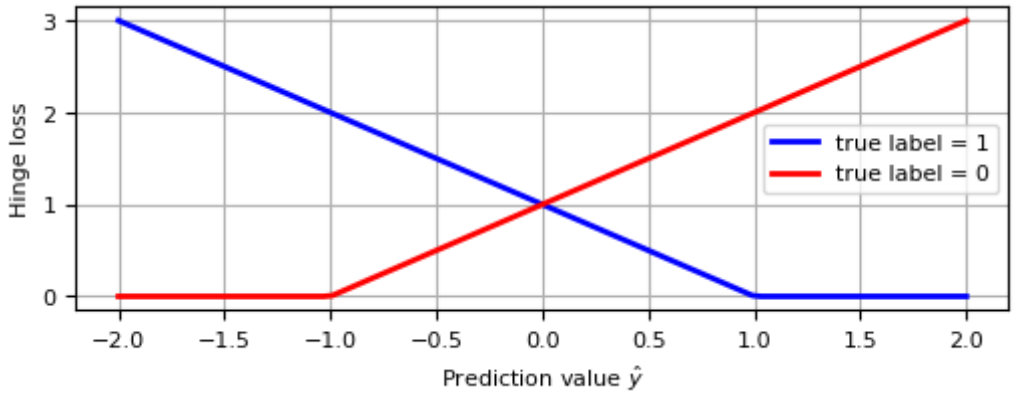
- If the data is not linearly separable, (hard) margin maximization becomes meaningless
- Relax the contraint by allowing an error ξ_i: $y_i(\mathbf{w}\mathbf{x_i} + w_0) \geq 1 - \xi_i$
- Or (since $\xi_i \geq 0$):

$$\xi_i = max(0, 1 - y_i \cdot (\mathbf{w}\mathbf{x_i} + w_0))$$

- The sum over all points is called *hinge loss*: $\sum_i^n \xi_i$
- Attenuating the error component with a hyperparameter C, we get the objective

$$\mathcal{L}(\mathbf{w}) = ||\mathbf{w}||^2 + C \sum_i^n \xi_i$$

- Can still be solved with quadratic programming

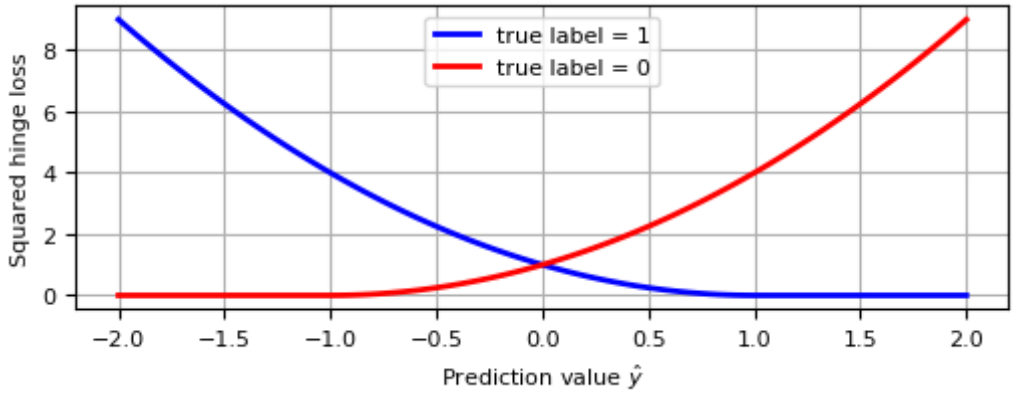


Least Squares SVMs

- We can also use the *squares* of all the errors, or squared hinge loss: $\sum_i^n \xi_i^2$
- This yields the Least Squares SVM objective

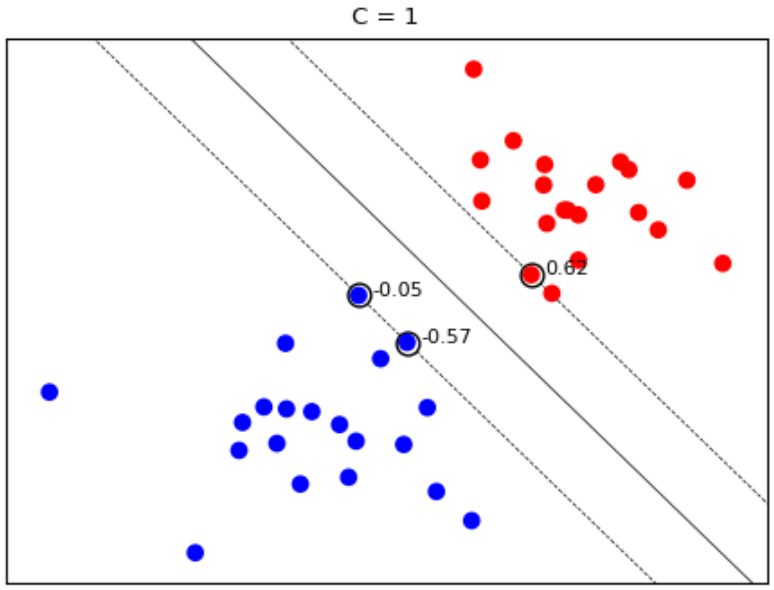
$$\mathcal{L}(\mathbf{w}) = ||\mathbf{w}||^2 + C \sum_i^n \xi_i^2$$

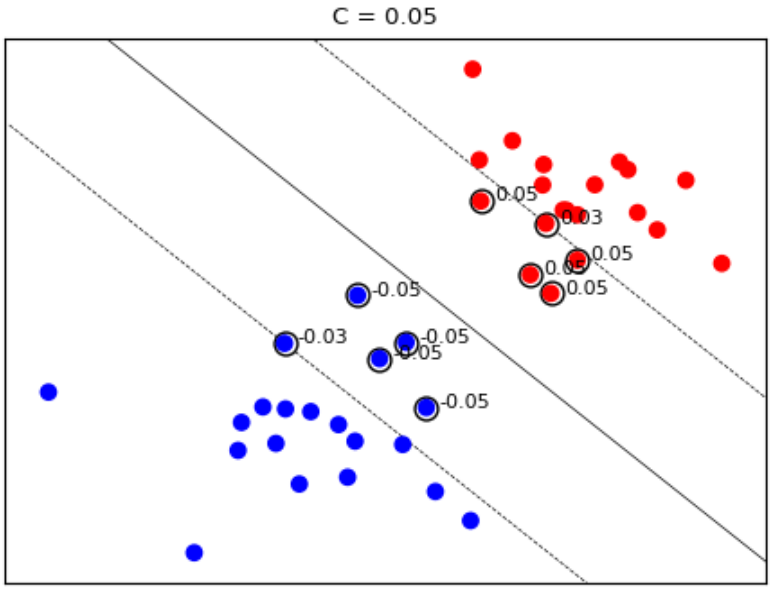
- Can be solved with Lagrangian Multipliers and a set of linear equations
  - Still yields support vectors and still allows kernelization
  - Support vectors are not sparse, but pruning techniques exist



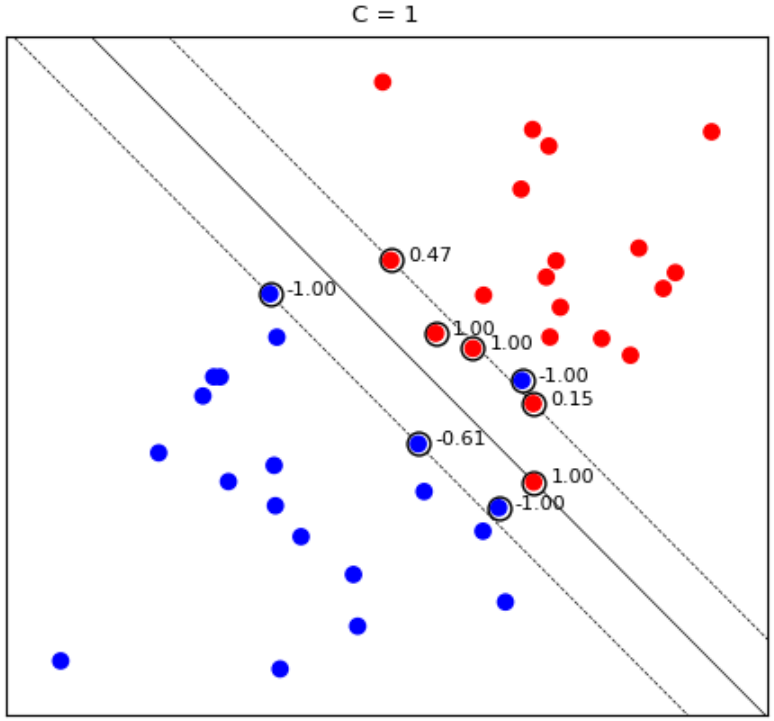
Effect of regularization on margin and support vectors

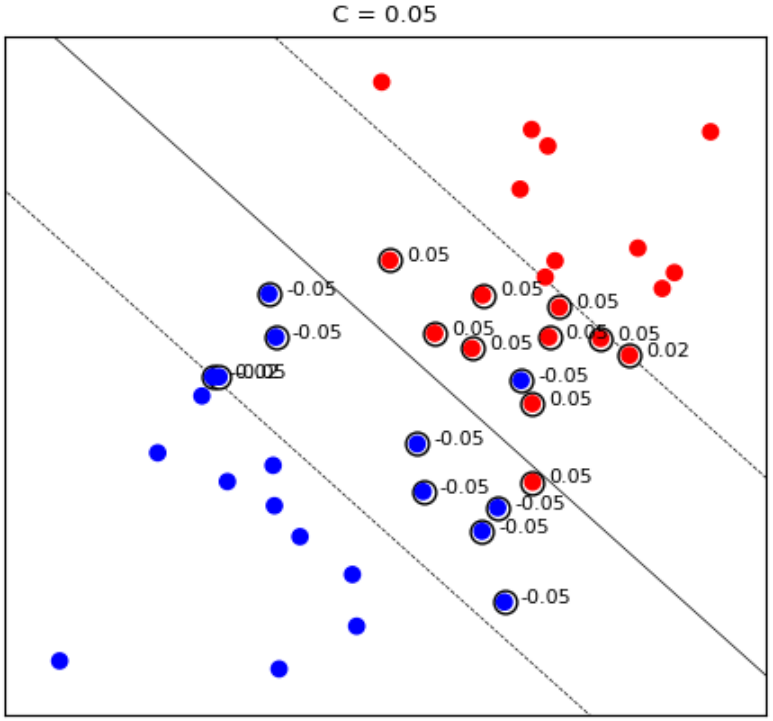
- SVM's Hinge loss acts like L1 regularization, yields sparse models
- C is the *inverse* regularization strength (inverse of α in Lasso)
  - Larger C: fewer support vectors, smaller margin, more overfitting
  - Smaller C: more support vectors, wider margin, less overfitting
- Needs to be tuned carefully to the data



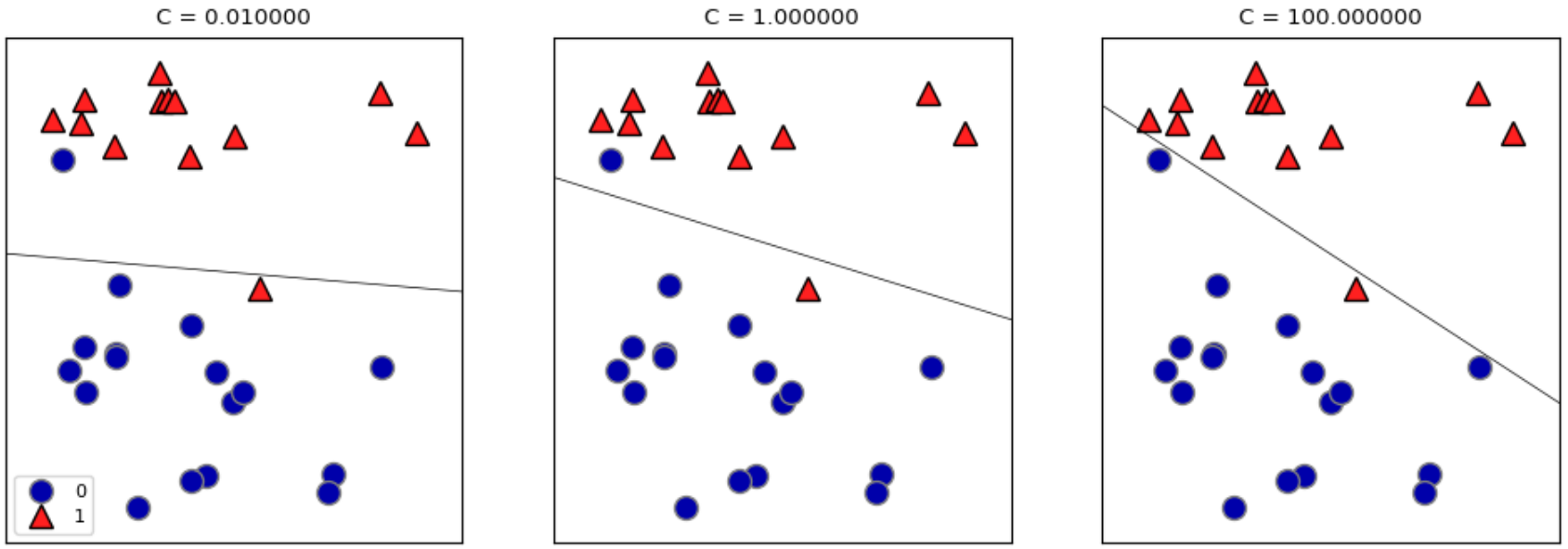


Same for non-linearly separable data





Large C values can lead to overfitting (e.g. fitting noise), small values can lead to underfitting



SVMs in scikit-learn

- `svm.LinearSVC`: faster for large datasets
  - Allows choosing between the primal or dual. Primal recommended when $n >> p$
  - Returns `coef_` ($\mathbf{w}$) and `intercept_` (w_0)
- `svm.SVC` with `kernel=linear`: allows *kernelization* (see later)
  - Also returns `support_vectors_` (the support vectors) and the `dual_coef_` a_i
  - Scales at least quadratically with the number of samples n
- `svm.LinearSVR` and `svm.SVR` are variants for regression

```
clf = svm.SVC(kernel='linear')
clf.fit(X, Y)
print("Support vectors:", clf.support_vectors_[:])
print("Coefficients:", clf.dual_coef_[:])
```

```
Support vectors:
[[-1.021  0.241]
 [-0.467 -0.531]
 [ 0.951  0.58 ]]
Coefficients:
[[-0.048 -0.569  0.617]]
```

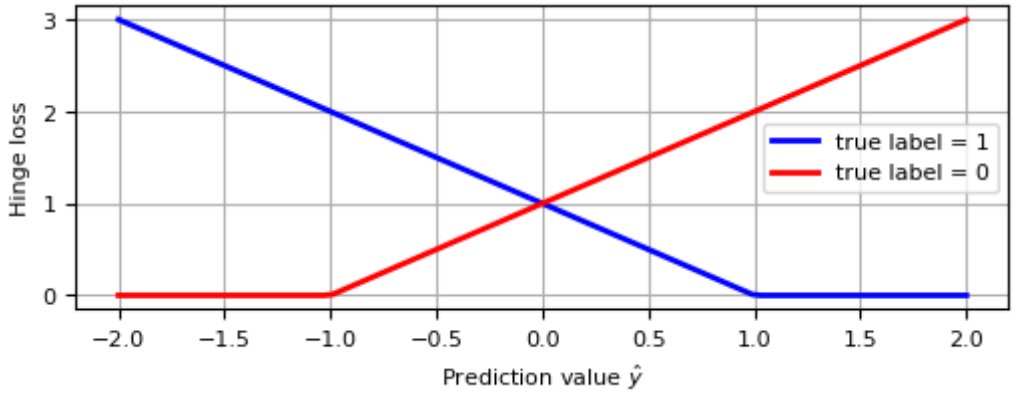
Solving SVMs with Gradient Descent

- Soft-margin SVMs can, alternatively, be solved using gradient decent
  - Good for large datasets, but does not yield support vectors or kernelization
- Squared Hinge is differentiable
- Hinge is not differentiable but convex, and has a subgradient:

$$\mathcal{L}_{Hinge}(\mathbf{w}) = max(0, 1 - y_i(\mathbf{wx_i} + w_0))$$

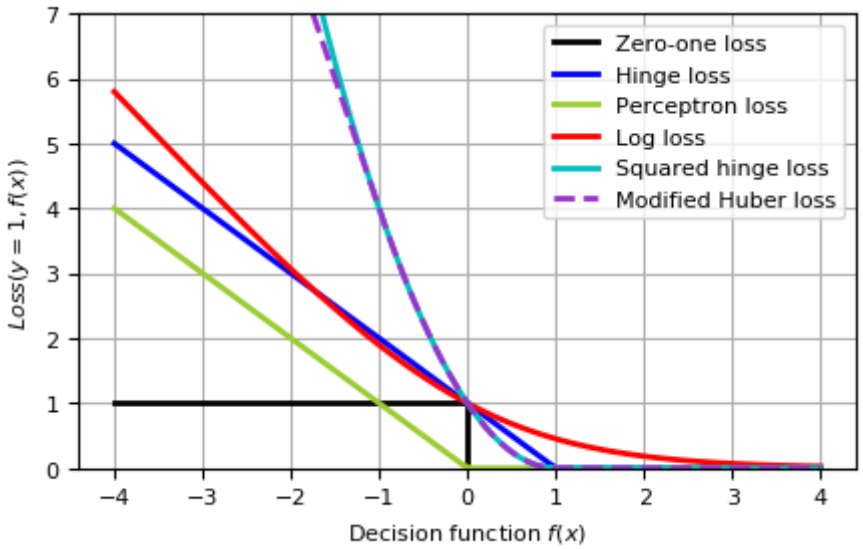
$$\frac{\partial \mathcal{L}_{Hinge}}{\partial w_i} = \begin{cases} -y_i x_i & y_i(\mathbf{wx_i} + w_0) < 1 \\ 0 & \text{otherwise} \end{cases}$$

- Can be solved with (stochastic) gradient descent



Generalized SVMs

- Because the derivative of hinge loss is undefined at y=1, smoothed versions are often used:
  - Squared hinge loss: yields *least squares SVM*
    - Equivalent to Ridge classification (with different solver)
  - Modified Huber loss: squared hinge, but linear after -1. Robust against outliers
- Log loss can also be used (equivalent to logistic regression)
- In sklearn, `SGDClassifier` can be used with any of these. Good for large datasets.

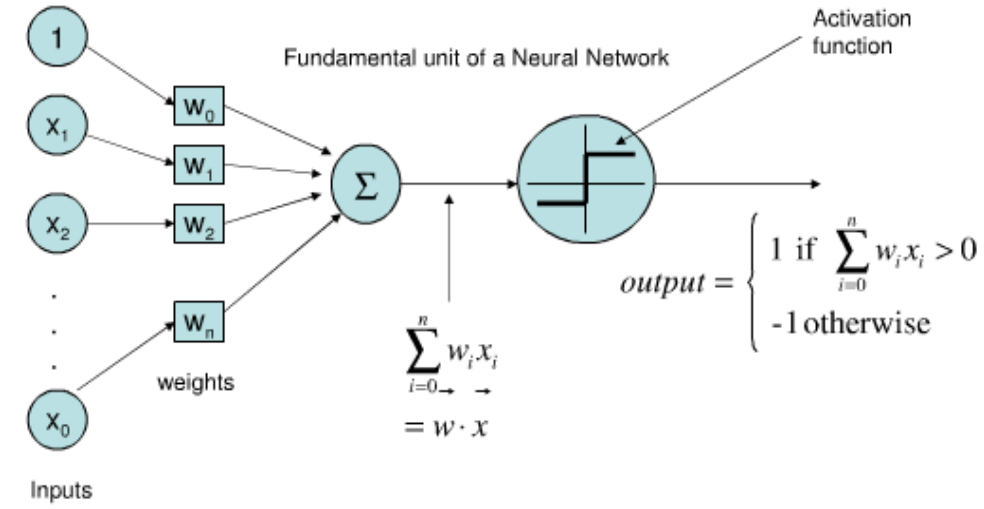


Perceptron

- Represents a single neuron (node) with inputs x_i, a bias w_0, and output y
- Each connection has a (synaptic) weight w_i. The node outputs
  $\hat{y} = \sum_i^n x_i w_i + w_0$
- The *activation function* predicts 1 if $\mathbf{xw} + w_0 > 0$, -1 otherwise
- Weights can be learned with (stochastic) gradient descent and Hinge(0) loss
  - Updated *only* on misclassification, corrects output by ± 1

$$\mathcal{L}_{Perceptron} = max(0, y_i(\mathbf{wx_i} + w_0))$$

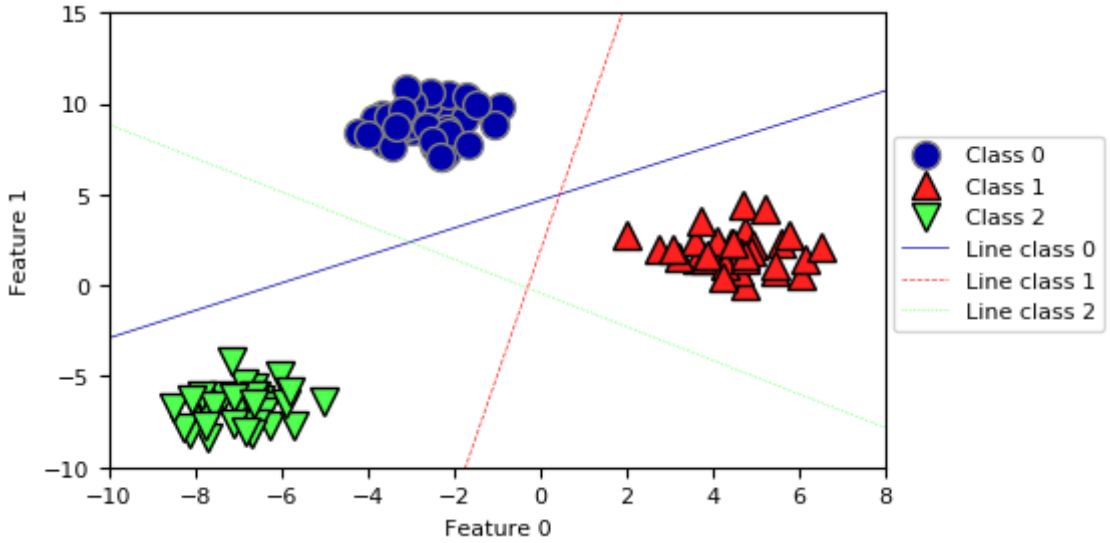
$$\frac{\partial \mathcal{L}_{Perceptron}}{\partial w_i} = \begin{cases} -y_i x_i & y_i(\mathbf{wx_i} + w_0) < 0 \\ 0 & \text{otherwise} \end{cases}$$



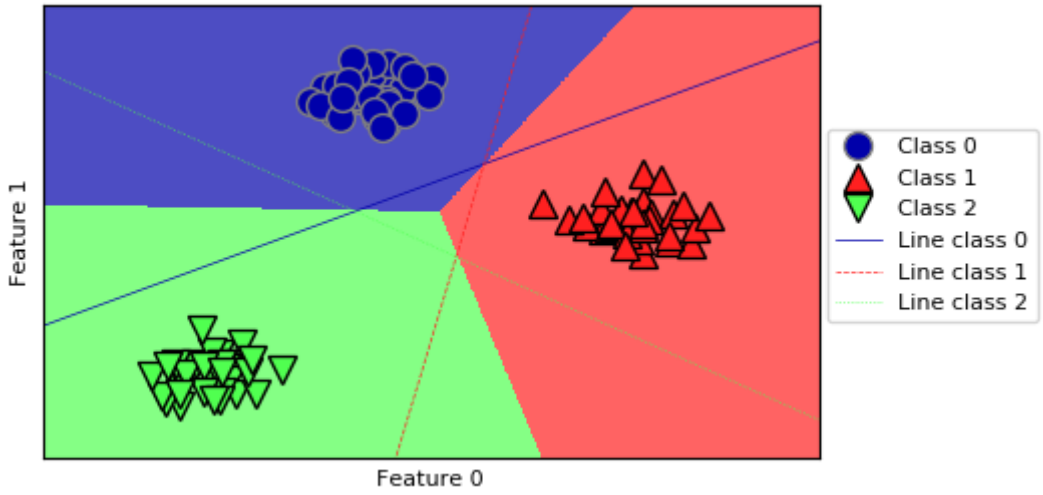
Linear Models for multiclass classification

one-vs-rest (aka one-vs-all)

- Learn a binary model for each class vs. all other classes
- Create as many binary models as there are classes



- Every binary classifiers makes a prediction, the one with the highest score (>0) wins



one-vs-one

- An alternative is to learn a binary model for every *combination* of two classes
  - For C classes, this results in $\frac{C(C-1)}{2}$ binary models
  - Each point is classified according to a majority vote amongst all models
  - Can also be a 'soft vote': sum up the probabilities (or decision values) for all models. The class with the highest sum wins.
- Requires more models than one-vs-rest, but training each one is faster
  - Only the examples of 2 classes are included in the training data
- Recommended for algorithms than learn well on small datasets
  - Especially SVMs and Gaussian Processes

Linear models overview

Name	Representation	Loss function	Optimization	Regularization
Least squares	Linear function (R)	SSE	CFS or SGD	None
Ridge	Linear function (R)	SSE + L2	CFS or SGD	L2 strength (α)
Lasso	Linear function (R)	SSE + L1	Coordinate descent	L1 strength (α)
Elastic-Net	Linear function (R)	SSE + L1 + L2	Coordinate descent	α, L1 ratio (ρ)
SGDRegressor	Linear function (R)	SSE, Huber, ϵ-ins,... + L1/L2	SGD	L1/L2, α
Logistic regression	Linear function (C)	Log + L1/L2	SGD, coordinate descent,...	L1/L2, α
Ridge classification	Linear function (C)	SSE + L2	CFS or SGD	L2 strength (α)
Linear SVM	Support Vectors	Hinge(1)	Quadratic programming or SGD	Cost (C)

Summary

- Linear models
  - Good for very large datasets (scalable)
  - Good for very high-dimensional data (not for low-dimensional data)
- Can be used to fit non-linear or low-dim patterns as well (see later)
  - Preprocessing: e.g. Polynomial or Poisson transformations
  - Generalized linear models (kernelization)
- Regularization is important. Tune the regularization strength (α)
  - Ridge (L2): Good fit, sometimes sensitive to outliers
  - Lasso (L1): Sparse models: fewer features, more interpretable, faster
  - Elastic-Net: Trade-off between both, e.g. for correlated features
- Most can be solved by different optimizers (solvers)
  - Closed form solutions or quadratic/linear solvers for smaller datasets
  - Gradient descent variants (SGD,CD,SAG,CG,...) for larger ones
- Multi-class classification can be done using a one-vs-all approach