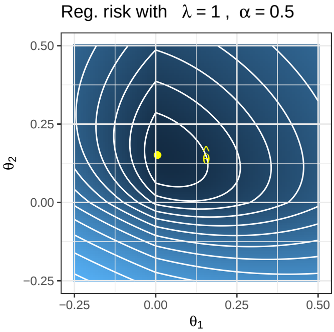
Optimization in Machine Learning

Optimization Problems: Unconstrained problems



Learning goals

- Definition
- Max. likelihood
- Linear regression
- Regularized risk minimization
- SVM
- Neural network

UNCONSTRAINED OPTIMIZATION PROBLEM

$$\min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x})$$

with objective function

$$f : \mathcal{S} \to \mathbb{R}.$$

The problem is called

- **unconstrained**, if the domain $\mathcal{S}$ is not restricted:

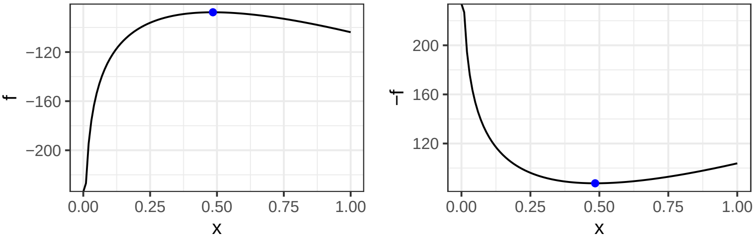
$$\mathcal{S} = \mathbb{R}^d$$

- **smooth** if f is at least $\in \mathcal{C}^1$
- **univariate** if $d = 1$, and **multivariate** if $d > 1$.
- **convex** if f convex function and $\mathcal{S}$ convex set

NOTE: A CONVENTION IN OPTIMIZATION

W.l.o.g., we always **minimize** functions f.

Maximization results from minimizing $-f$.



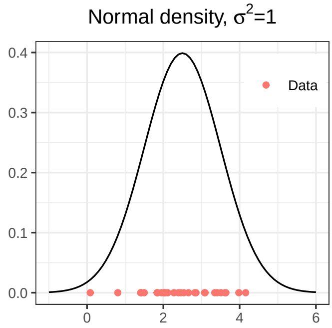
The solution to maximizing f (left) is equivalent to the solution to minimizing f (right).

EXAMPLE 1: MAXIMUM LIKELIHOOD

$\mathcal{D} = \left(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right) \overset{\text{i.i.d.}}{\sim} f(\mathbf{x} \mid \mu, \sigma)$ with $\sigma = 1$:

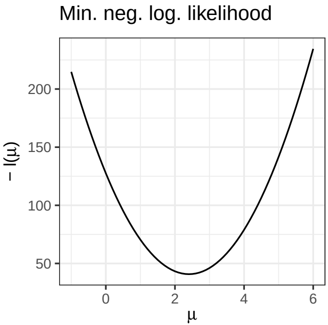
$$f(\mathbf{x} \mid \mu, \sigma) = \frac{1}{\sqrt{2\mu\sigma^2}} \exp\left(\frac{-(\mathbf{x} - \mu)^2}{2\sigma^2}\right)$$

Goal: Find $\mu \in \mathbb{R}$ which makes observed data most likely.



EXAMPLE 1: MAXIMUM LIKELIHOOD

- **Likelihood:**
$$\mathcal{L}(\mu \mid \mathcal{D}) = \prod_{i=1}^{n} f\left(\mathbf{x}^{(i)} \mid \mu, 1\right) = (2\pi)^{-n/2} \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}^{(i)} - \mu)^2\right)$$
- **Neg. log-likelihood:**
$$-\ell(\mu, \mathcal{D}) = -\log \mathcal{L}(\mu \mid \mathcal{D}) = \frac{n}{2}\log(2\pi) + \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}^{(i)} - \mu)^2$$

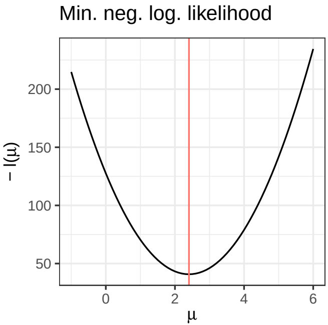


EXAMPLE 1: MAXIMUM LIKELIHOOD

$$\min_{\mu \in \mathbb{R}} -\ell(\mu, \mathcal{D}).$$

can be solved analytically (setting the first deriv. to 0) since it is a quadratic form:

$$-\frac{\partial \ell(\mu, \mathcal{D})}{\partial \mu} = \sum_{i=1}^{n} \left(\mathbf{x}^{(i)} - \mu\right) \quad = \quad 0 \quad \Leftrightarrow \quad \hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}^{(i)}$$



EXAMPLE 1: MAXIMUM LIKELIHOOD

Note: The problem was **smooth**, **univariate**, **unconstrained**, **convex**.

If we had optimized for σ as well

$$\min_{\mu \in \mathbb{R}, \sigma \in \mathbb{R}^+} -\ell(\mu, \mathcal{D}).$$

(instead of assuming it is known) the problem would have been:

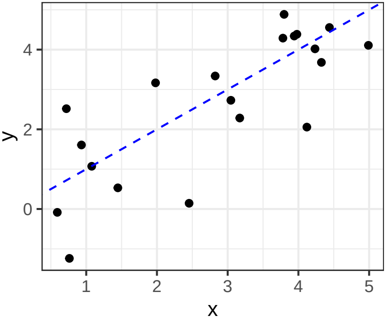
- bivariate (optimize over (μ, σ))
- constrained ($\sigma > 0$)

$$\min_{\mu \in \mathbb{R}, \sigma \in \mathbb{R}^+} -\ell(\mu, \mathcal{D}).$$

EXAMPLE 2: NORMAL REGRESSION

Assume (multivariate) data $\mathcal{D} = \left(\left(\mathbf{x}^{(1)}, y^{(1)}\right), \dots, \left(\mathbf{x}^{(n)}, y^{(n)}\right)\right)$ and we want to fit a linear function to it

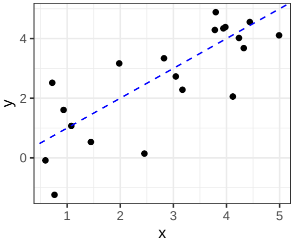
$$y = f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}$$

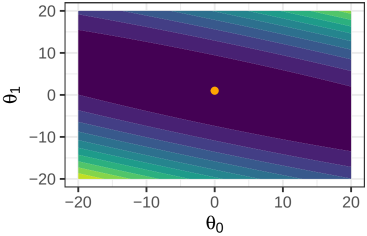


EXAMPLE 2: LEAST SQUARES LINEAR REGR.

Find param vector $\boldsymbol{\theta}$ that minimizes SSE / risk with L2 loss

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \sum_{i=1}^{n} \left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - y^{(i)} \right)^2$$





- **Smooth**, **multivariate**, **unconstrained**, **convex** problem
- Quadratic form
- Analytic solution: $\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y}$, where $\mathbf{X}$ is design matrix

RISK MINIMIZATION IN ML

In the above example, if we exchange

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \sum_{i=1}^{n} \left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - y^{(i)} \right)^2$$

- the linear model $\boldsymbol{\theta}^\top \mathbf{x}$ by an arbitrary model $f(\mathbf{x} \mid \boldsymbol{\theta})$
- the L2-loss $(f(\mathbf{x} \mid \boldsymbol{\theta}) - y)^2$ by any loss $L(y, f(\mathbf{x}))$

we arrive at general **empirical risk minimization** (ERM)

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) = \min!$$

Usually, we add a regularizer to counteract overfitting:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) + \lambda J(\boldsymbol{\theta}) = \min!$$

RISK MINIMIZATION IN ML

ML models usually consist of the following components:

$$\textbf{ML} = \underbrace{\textbf{Hypothesis Space + Risk + Regularization}}_{\text{Formulating the optimization problem}} + \underbrace{\textbf{Optimization}}_{\text{Solving it}}$$

- **Hypothesis Space:** Parametrized function space
- **Risk:** Measure prediction errors on data with loss L
- **Regularization:** Penalize model complexity
- **Optimization:** Practically minimize risk over parameter space

EXAMPLE 3: REGULARIZED LM

ERM with L2 loss, LM, and L2 regularization term:

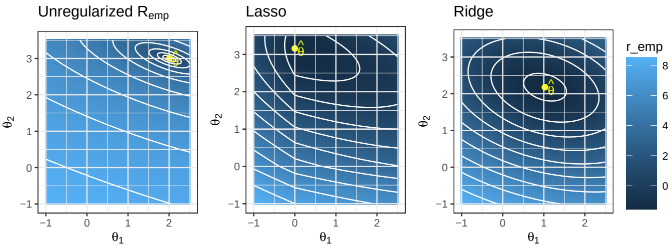
$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - y^{(i)}\right)^2 + \lambda \cdot \|\boldsymbol{\theta}\|_2^2 \quad \text{(Ridge regr.)}$$

Problem **multivariate**, **unconstrained**, **smooth**, **convex** and has analytical solution $\boldsymbol{\theta} = (\mathbf{X}^\top \mathbf{X} + \lambda \boldsymbol{I})^{-1} \mathbf{X}^\top \boldsymbol{y}$.

ERM with L2-loss, LM, and L1 regularization:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - y^{(i)}\right)^2 + \lambda \cdot \|\boldsymbol{\theta}\|_1 \quad \text{(Lasso regr.)}$$

The problem is still **multivariate**, **unconstrained**, **convex**, but **not smooth**.

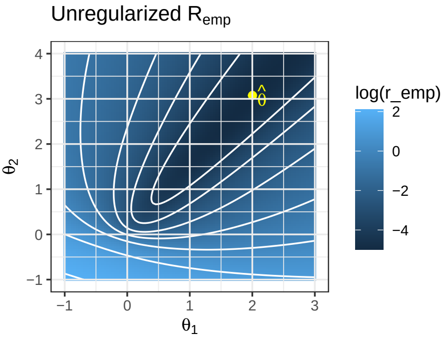


EXAMPLE 4: (REGULARIZED) LOG. REGRESSION

For $y \in \{0, 1\}$ (classification), logistic regression minimizes log / Bernoulli / cross-entropy loss over data

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(-y^{(i)} \cdot \boldsymbol{\theta}^\top \mathbf{x}^{(i)} + \log\left(1 + \exp\left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)}\right)\right)\right)$$

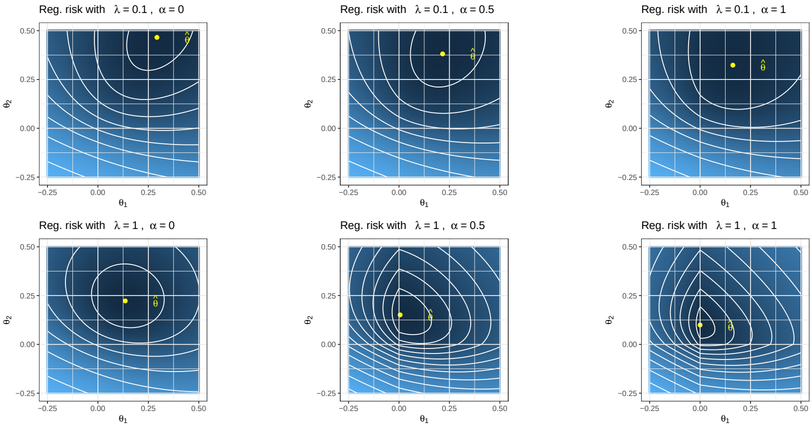
Multivariate, unconstrained, smooth, convex, not analytically solvable.



EXAMPLE 4: (REGULARIZED) LOG. REGRESSION

Elastic net regularization is a combination of L1 and L2 regularization

$$\frac{1}{2n}\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) + \lambda\left[\frac{1-\alpha}{2}\|\theta\|_2^2 + \alpha\|\theta\|_1\right], \lambda \geq 0, \alpha \in [0,1]$$



The higher λ, the closer to the origin, L1 shrinks coeffs exactly to 0.

EXAMPLE 4: (REGULARIZED) LOG. REGRESSION

$$\frac{1}{2n}\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) + \lambda\left[\frac{1-\alpha}{2}\|\theta\|_2^2 + \alpha\|\theta\|_1\right], \lambda \geq 0, \alpha \in [0,1]$$

Problem characteristics:

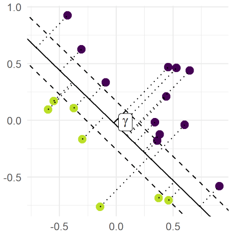
- Multivariate
- Unconstrained
- If $\alpha = 0$ (Ridge) problem is smooth; not smooth otherwise
- Convex since *L* convex and both L1 and L2 norm are convex

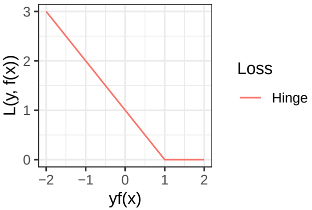
EXAMPLE 5: LINEAR SVM

- $\mathcal{D} = \left(\left(\mathbf{x}^{(i)}, y^{(i)}\right)\right)_{i=1,\ldots,n}$ with $y^{(i)} \in \{-1, 1\}$ (classification)
- $f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \mathbf{x} \in \mathbb{R}$ scoring classifier:
  Predict 1 if $f(\mathbf{x} \mid \boldsymbol{\theta}) > 0$ and -1 otherwise.

ERM with LM, hinge loss, and L2 regularization:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \max\left(1 - y^{(i)} f^{(i)}, 0\right) + \lambda \boldsymbol{\theta}^\top \boldsymbol{\theta}, \quad f^{(i)} := \boldsymbol{\theta}^\top \mathbf{x}^{(i)}$$



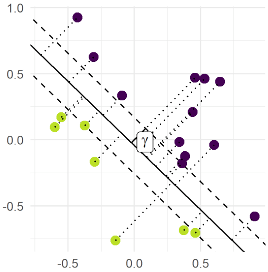


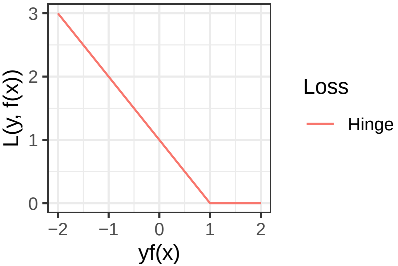
This is one formulation of the **linear SVM**. Problem is: **multivariate**, **unconstrained**, **convex**, but **not smooth**.

EXAMPLE 5: LINEAR SVM

Understanding hinge loss $L(y, f(\mathbf{x})) = \max(1 - y \cdot f, 0)$

y	$f(\mathbf{x})$	**Correct pred.?**	$L(y, f(\mathbf{x}))$	**Reason for costs**
1	$(-\infty, 0)$	N	$(1, \infty)$	Misclassification
-1	$(0, \infty)$	N	$(1, \infty)$	Misclassification
1	$(0, 1)$	Y	$(0, 1)$	Low confidence / margin
-1	$(-1, 0)$	Y	$(0, 1)$	Low confidence / margin
1	$(1, \infty)$	Y	0	–
-1	$(-\infty, -1)$	Y	0	–





EXAMPLE 6: KERNELIZED SVM

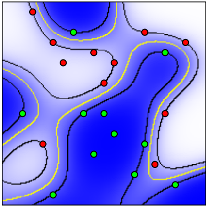
Kernelized formulation of the primal$^{(*)}$ SVM problem:

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} L\left(y^{(i)}, \boldsymbol{K}_i^\top \boldsymbol{\theta}\right) + \lambda \boldsymbol{\theta}^\top \boldsymbol{K} \boldsymbol{\theta}$$

with $k(\cdot, \cdot)$ pos. def. kernel function, and
$\boldsymbol{K}_{ij} := k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$, $n \times n$ psd kernel matrix, $\boldsymbol{K}_i$ i-th column of K.

Kernelization

- allows introducing nonlinearity through projection into higher-dim. feature space
- without changing problem characteristics (convexity!)



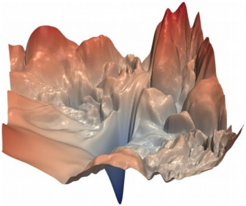
$^{(*)}$ There is also a dual formulation to the problem (comes later!)

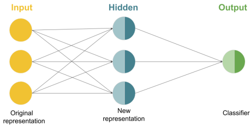
EXAMPLE 6: NEURAL NETWORK

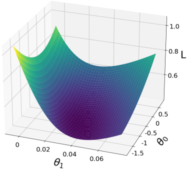
Normal loss, but complex f defined as computational feed-forward graph. Complexity of optimization problem

$$\arg\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}),$$

so smoothness (maybe) or convexity (usually no) is influenced by loss, neuron function, depth, regularization, etc.







Loss landscapes of ML problems.

Left: Deep learning model ResNet-56, right: Logistic regression with cross-entropy loss

Source: `https://arxiv.org/pdf/1712.09913.pdf`