Statistical Data Analysis

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Ill-posedness and Regularization

If the least squares problem is ill-posed, i.e., solution does not exist or is unstable.

Small perturbations in $\mathbf{y}$ or $\mathbf{X}$ yield large perturbations in β

Solve regularized problem: For some $\lambda > 0$ and matrix $\mathbf{G}$

$$\min_{\beta} \frac{1}{2}\|\mathbf{X}\beta - \mathbf{y}^\top\|^2 + \frac{\lambda}{2}\|\mathbf{G}\beta\|^2$$

Iterative Methods

Iterative Solvers for Least-Squares Regression

So far: Given $\mathbf{y} \in \mathbb{R}^n$, solve

$$\min_{\beta} \frac{1}{2} \|\mathbf{X}\beta - \mathbf{y}\|$$

directly using $\beta^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}^\top$. Here

$$\mathbf{X} \in \mathbb{R}^{n \times (p+1)} \quad \text{and} \quad \beta \in \mathbb{R}^{(p+1)}.$$

Problems:

1. Generating $\mathbf{X}^\top \mathbf{X}$ and solving normal equations is too costly for large-scale problems.
2. Exact solution not useful when problem is ill-posed $\rightsquigarrow$ add explicit regularization or do so implicitly by early stopping.

Iterative methods that avoid working with $\mathbf{X}^\top \mathbf{X}$

- Steepest descent
- Conjugate gradient for least-squares (CGLS)

Excellent references: Numerical Optimization [4], iterative linear algebra [5], general introduction [1]

Iterative Methods

General idea - obtain a sequence $\beta_1, \ldots, \beta_j, \ldots$ that converges to least-squares solution β^*

$$\beta_j \longrightarrow \beta^*, \quad \text{for} \quad j \to \infty.$$

How fast does the sequence converge? Assume

$$\|\beta_{j+1} - \beta^*\| < \gamma_j \|\beta_j - \beta^*\|$$

where all $\gamma_j < 1$. Then

- If γ_j is bounded away from 0 and 1 the convergence is linear
- If $\gamma_j \to 0$ the convergence is superlinear
- If $\gamma_j \to 1$ the convergence is sublinear

The sequence converges quadratically if γ_j is bounded away from 0 and 1 and

$$\|\beta_{j+1} - \beta^*\| < \gamma_j \|\beta_j - \beta^*\|^2$$

Steepest Descent for Least-Squares

Consider now

$$\phi(\beta) = \frac{1}{2}\|\mathbf{X}\beta - \mathbf{y}\|^2 \quad \text{with} \quad \nabla_\beta \phi(\beta) = \mathbf{X}^\top(\mathbf{X}\beta - \mathbf{y}).$$

Steepest descent direction is $\mathbf{d}_j = \mathbf{X}^\top(\mathbf{y} - \mathbf{X}\beta_j)$ and

$$\beta_{j+1} = \beta_j + \alpha_j \mathbf{d}_j$$

How to choose α_j?

Idea: Minimize ϕ along direction $\mathbf{d}_j$

$$\alpha_j = \operatorname*{argmin}_\alpha \phi(\beta_j + \alpha \mathbf{d}_j) = \operatorname*{argmin}_\alpha \frac{1}{2}\|\alpha \mathbf{X}\mathbf{d}_j - \mathbf{r}_j\|^2$$

with residual $\mathbf{r}_j = \mathbf{y} - \mathbf{X}\beta_j$.

This leads to simple quadratic equation in 1D whose solution is

$$\alpha_j = \frac{\mathbf{r}_j^\top \mathbf{X}\mathbf{d}_j}{\|\mathbf{X}\mathbf{d}_j\|^2}$$

Algorithm: Steepest Descent for Least-Squares

for $j = 1, \ldots$

- Compute residual $\mathbf{r}_j = \mathbf{y} - \mathbf{X}\beta_j$
- Compute the SD direction $\mathbf{d}_j = \mathbf{X}^\top \mathbf{r}_j$
- Compute step size $\alpha_j = \frac{\mathbf{r}_j^\top \mathbf{X}\mathbf{d}_j}{\|\mathbf{X}\mathbf{d}_j\|^2}$
- Take the step $\beta_{j+1} = \beta_j + \alpha_j \mathbf{d}_j$

Converges linearly, i.e.,

$$\|\beta_{j+1} - \beta^*\| < \gamma \|\beta_j - \beta^*\| \quad \text{with} \quad \gamma \approx \left|\frac{\kappa - 1}{\kappa + 1}\right|$$

Here, κ depends on condition number of $\mathbf{X}$, i.e.,

$$\kappa \approx \frac{\sigma_{\mathbf{max}}^2}{\sigma_{\mathbf{min}}^2}$$

Can be painfully slow for ill-conditioned problems

Accelerating Steepest Descent: Post-Conditioning

Idea: Improve convergence by transforming the problem

$$\phi(\beta) = \frac{1}{2}\|\mathbf{XSS}^{-1}\beta - \mathbf{y}\|^2$$

Here: $\mathbf{S}$ is invertible
Solve in two steps:

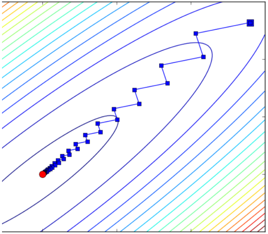
1. Set $\mathbf{z} = \mathbf{S}^{-1}\beta$ and compute

$$\mathbf{z}^* = \underset{\mathbf{z}}{\operatorname{argmin}} \frac{1}{2}\|\mathbf{XSz} - \mathbf{y}\|^2$$

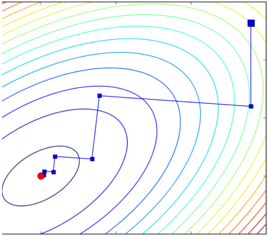
2. Then $\beta = \mathbf{Sz}$.

Pick $\mathbf{S}$ such that $\mathbf{XS}$ is better conditioned.

original problem:



post-conditioned:



Conjugate Gradient Method for Least-Squares

CG is designed to solve quadratic optimization problems

$$\min_{\beta} \frac{1}{2}\beta^\top \mathbf{H}\beta - \mathbf{b}^\top \beta$$

with $\mathbf{H}$ symmetric positive definite. In our case

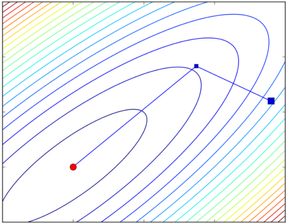
$$\underset{\beta}{\operatorname{argmin}} \frac{1}{2}\|\mathbf{X}\beta - \mathbf{y}\|^2 = \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\beta^\top \underbrace{\mathbf{X}^\top \mathbf{X}}_{=\mathbf{H}} \beta - \underbrace{\mathbf{y}^\top \mathbf{X}}_{=\mathbf{b}^\top} \beta$$

CG improves over SD by using previous step (not a memory-less method) and constructing a basis for the solution.

Facts:

- terminates after at most n steps (in exact arithmetic)
- good solutions for $j \ll n$
- convergence $\gamma_j \approx \left|\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right|^j$

Conjugate Gradient Least-Squares



- Uses the structure of the problem to obtain stable implementation
- Typically converges much faster than SD
- Accelerate using post conditioning

$$\min_{\beta} \frac{1}{2} \|\mathbf{X}\mathbf{S}\mathbf{S}^{-1}\beta - \mathbf{y}\|^2$$

- Faster convergence when eigenvalues of $\mathbf{S}^\top \mathbf{X}^\top \mathbf{X}\mathbf{S}$ are clustered.

Iterative Regularization

Consider

$$\min_{\beta} \|\mathbf{X}\beta - \mathbf{b}\|^2$$

- Assume that $\mathbf{X}$ has non-trivial null space
- The matrix $\mathbf{X}^\top \mathbf{X}$ is not invertible
- Can we still use iterative methods (CG, CGLS, ...)?

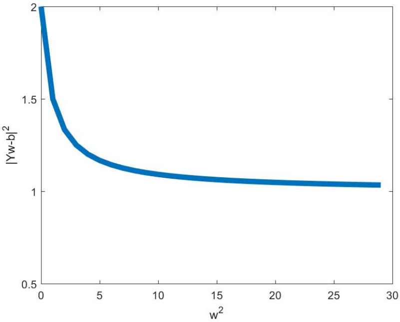
What are the properties of the iterates?

Excellent introduction to computational inverse problems [2, 6, 3]

Iterative Regularization: L-Curve

The CGLS algorithm has the following properties

- For each iteration $\|\mathbf{X}\beta_k - \mathbf{y}\|^2 \leq \|\mathbf{X}\beta_{k-1} - \mathbf{y}\|^2$
- If starting from $\beta = 0$ then $\|\beta_k\|^2 \geq \|\beta_{k-1}\|^2$
- $\beta_1, \beta_2, \ldots$ converges to the minimum norm solution of the problem
- Plotting $\|\beta_k\|^2$ vs $\|\mathbf{X}\beta_k - \mathbf{y}\|^2$ typically has the shape of an L-curve



Cross Validation - 1

Finding good least-squares solution requires good parameter selection.

- λ when using Tikhonov regularization (weight decay)
- number of iteration (for SD and CGLS)

Suppose that we have two different "solutions"

$$\begin{aligned} \beta_1 \quad &\rightarrow \quad \|\beta_1\|^2 = \eta_1 \quad \|\mathbf{X}\beta_1 - \mathbf{y}\|^2 = \rho_1. \\ \beta_2 \quad &\rightarrow \quad \|\beta_2\|^2 = \eta_2 \quad \|\mathbf{X}\beta_2 - \mathbf{y}\|^2 = \rho_2. \end{aligned}$$

How to decide which one is better?

Cross Validation - 2

Goal: Gauge how well the model can predict new examples.

Let $\{\mathbf{X}_{\mathrm{CV}}, \mathbf{y}_{\mathrm{CV}}\}$ be data that is **not used** for the training

Idea: If $\|\mathbf{X}_{\mathrm{CV}}\beta_1 - \mathbf{y}_{\mathrm{CV}}\|^2 \leq \|\mathbf{X}_{\mathrm{CV}}\beta_2 - \mathbf{y}_{\mathrm{CV}}\|^2$, then β_1 is a better solution that β_2.

When the solution depends on some hyper-parameter(s) λ, we can phrase this as bi-level optimization problem

$$\lambda^* = \operatorname*{argmin}_{\lambda} \|\mathbf{X}_{\mathrm{CV}}\beta(\lambda) - \mathbf{y}_{\mathrm{CV}}\|^2,$$

where $\beta(\lambda) = \operatorname{argmin}_\beta \frac{1}{2}\|\mathbf{X}\beta - \beta\|^2 + \frac{\lambda}{2}\|\beta\|^2$.

Cross Validation - 3

To assess the final quality of the solution cross validation is not sufficient (why?).

Need a final testing set.

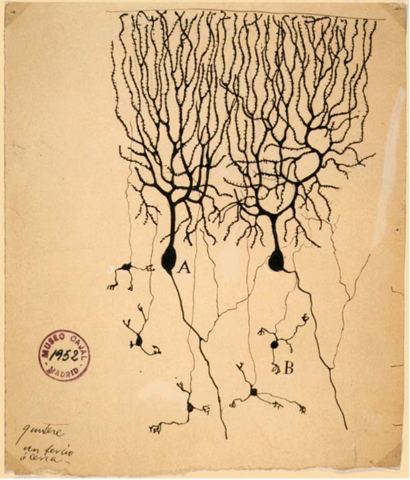
Procedure

- Divide the data into 3 groups $\{\mathbf{X}_{\text{train}}, \mathbf{X}_{\text{CV}}, \mathbf{X}_{\text{test}}\}$.
- Use $\mathbf{X}_{\text{train}}$ to estimate $\beta(\lambda)$
- Use $\mathbf{X}_{\text{CV}}$ to estimate λ
- Use $\mathbf{X}_{\text{test}}$ to assess the quality of the solution

Important - we are not allowed to use $\mathbf{X}_{\text{test}}$ to tune parameters!

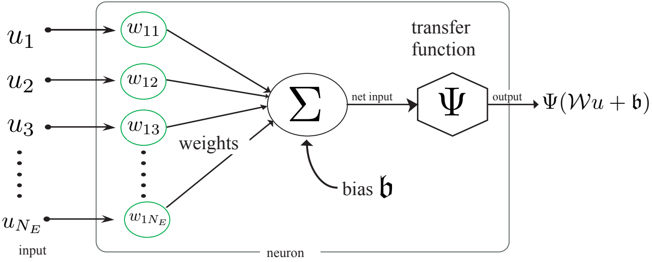
Neural Networks

Motivation from biology



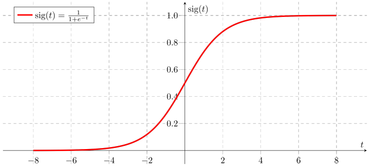
By Santiago Ramn y Cajal in 1899 see
https://de.wikipedia.org/wiki/Santiago_Ramn_y_Cajalfordetails

Neuron



u_1
u_2
u_3
u_{N_E}
input
w_{11}
w_{12}
w_{13}
w_{1N_E}
weights
$\sum$
net input
transfer function
Ψ
output
$\Psi(\mathcal{W}u + \mathfrak{b})$
bias $\mathfrak{b}$
neuron

Activation function example: sigmoid



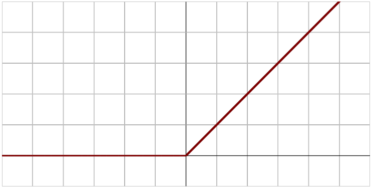
Sigmoid function:

$\mathrm{sig}(t) = \frac{1}{1+e^{-t}}$

Properties:

- Derivative: $\dfrac{1 + e^{-x} + xe^{-x}}{\left(1 + e^{-x}\right)^2}$
- $\mathrm{sig}'(t) = \mathrm{sig}(t)\,(1 - \mathrm{sig}(t))$

Activation function example: ReLu



Rectified linear unit:

$$\text{ReLu}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$$
$$= \max\{0, x\}$$

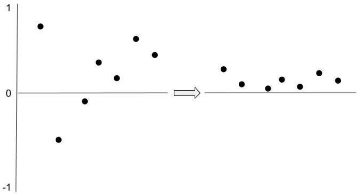
Properties:

- Derivative:

$$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0 \end{cases} \tag{1}$$

- very popular for Deep RL
- Dying ReLU problem - vanishing gradient problem.

Activation function example: Softmax



Softmax:

$$\sigma(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}} \qquad \text{for } i = 1, \ldots, K$$

and $\mathbf{z} = (z_1, \ldots, z_K) \in \mathbb{R}^K$.

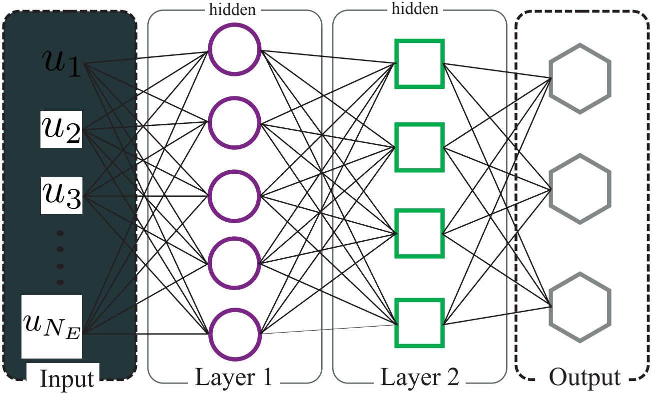
Properties:

- Derivative:

$$\frac{\partial}{\partial q_k} \sigma(\mathbf{q}, i) = \sigma(\mathbf{q}, i)(\delta_{ik} - \sigma(\mathbf{q}, k)). \tag{2}$$

- used in to normalize the output (map to a probability distribution)
- also used in RL to convert action values into action probabilities

Multilayer perceptron



Training Neural Network

1. Choose network architecture:
    - activation functions
    - hidden layers (shallow or deep)
    - number of neurons
    - etc.
2. Choose appropriate loss function E, e.g., least squares
3. Find minima via:
    - stochastic gradient descent
    - Backpropagation

Stochastic Gradient Descent

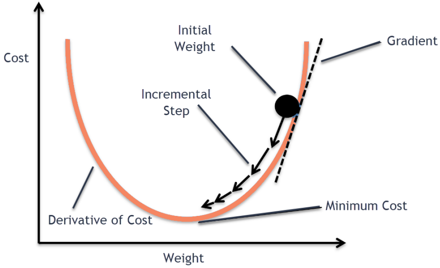


Image ref: https://morioh.com/p/bc6bc20e9739 and https://medium.com/38th-street-studios/exploring-stochastic-gradient-descent-with-restarts-sgdr-fa206c38a74e

Iterative weight improvement:

$$w := w - \eta \nabla E_i(w). \tag{3}$$

Backpropagation

Backpropagation

Backpropagation

Backpropagation

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