

# Coordinate descent

Alexandre Gramfort

[alexandre.gramfort@inria.fr](mailto:alexandre.gramfort@inria.fr)



Master 2 Data Science, Univ. Paris Saclay  
Optimisation for Data Science  
*course based on notes from Olivier Fercoq.*

# Table of Contents

- 1 Exact coordinate descent
- 2 Coordinate gradient descent
- 3 Proximal coordinate descent
- 4 Applications to ML estimators

# Why coordinate descent for datascience?

So far you have seen first order method:

- gradient descent
- proximal gradient descent
- accelerated gradient descent

You'll also see with me

- Newton methods
- quasi-Newton methods

Coordinate descent (CD) has received a lot of attention in ML/stats over the last 10 years. It's state-of-the-art techniques on a number of learning problems, as CD applies in this settings (not as general as gradient descent). It's what R GLMNET package and Scikit-Learn Lasso / Elastic-Net / LinearSVC estimators use.

# Coordinate wise optimization

We work in finite dimension  $\mathbb{R}^n$  (think  $n$  parameters to optimize)

Coordinate descent is **extremely simple**

**Idea:** minimize one coordinate at a time (keeping the other fixed)

**Question:** Given convex, differentiable  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , if we are at a point  $x$  such that  $f(x)$  is minimized along each coordinate axis, have we found a global minimizer?

i.e., does  $f(x + dU_i) \geq f(x) \forall d \in \mathbb{R}, \forall i \Rightarrow f(x) = \min_z f(z)$ ?

where  $U_i = (0, \dots, 1, \dots, n) \in \mathbb{R}^n$  is the  $i$ th canonical basis vector.

# Coordinate wise optimization

$f(x + dU_i) \geq f(x), \forall d \in \mathbb{R}$  implies that

$$\frac{\partial f}{\partial x^{(i)}}(x) = 0$$

which implies

$$\nabla f(x) = \left( \frac{\partial f}{\partial x^{(1)}}(x), \dots, \frac{\partial f}{\partial x^{(n)}}(x) \right) = 0$$

OK for  $f$  smooth and convex !

# Table of Contents

- 1 Exact coordinate descent
- 2 Coordinate gradient descent
- 3 Proximal coordinate descent
- 4 Applications to ML estimators

# Exact coordinate descent

Objective:  $\min_{x \in \mathbb{R}^n} f(x)$

Initialisation:  $x_0 = (x_0^{(1)}, \dots, x_0^{(n)})$ .

Algorithm:

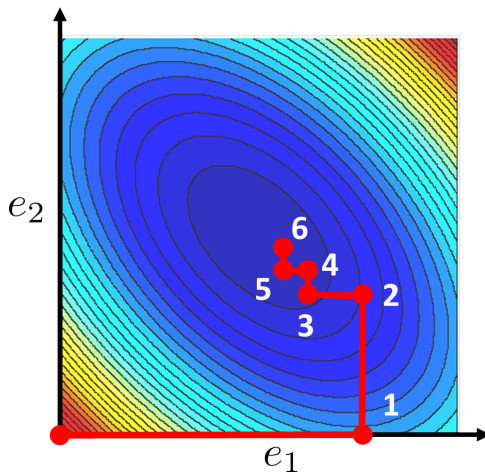
Choose  $l = (k \bmod n) + 1$  (cyclic rule)

$$\begin{cases} x_{k+1}^{(i)} = \arg \min_{z \in \mathbb{R}} f(x_k^{(1)}, \dots, x_k^{(l-1)}, z, x_k^{(l+1)}, \dots, x_k^{(n)}) & \text{if } i = l \\ x_{k+1}^{(i)} = x_k^{(i)} & \text{if } i \neq l \end{cases}$$

**Note:** The order of cycle through coordinates is arbitrary, can use any permutation of  $1, 2, \dots, n$ .

**Note:** We just have to solve 1D optimization problems but a lot of them...

# Example



Coordinate descent on a 2D problem



# Example: Linear regression

Let  $f(x) = \frac{1}{2} \|y - Ax\|^2$ , where  $y \in \mathbb{R}^m$ ,  $A \in \mathbb{R}^{m \times n}$  is the design matrix with columns  $A_1, \dots, A_n$  (one per feature)

Consider minimizing over  $x^{(i)}$ , with all  $x^{(j)}$ ,  $j \neq i$  fixed:

$$0 = \nabla_i f(x) = A_i^\top (Ax - y) = A_i^\top (A_i x^{(i)} + A_{-i} x^{(-i)} - y)$$

i.e., we take:

$$x^{(i)} = \frac{A_i^\top (y - A_{-i} x^{(-i)})}{A_i^\top A_i}$$

Repeat these update by cycling over coordinates

→ notebook

# Example: Linear regression

Note that doing:

$$x^{(i)} = \frac{A_i^\top (y - A_{-i} x^{(-i)})}{A_i^\top A_i}$$

is equivalent to:

$$x^{(i)} \leftarrow x^{(i)} + \frac{A_i^\top r}{A_i^\top A_i}$$

where  $r = y - Ax$  is the current *residual*. If current  $r$  is available the cost of an update is  $O(m)$ . Updating  $r$  is also  $O(m)$  so full pass/epoch on coordinates is  $O(mn)$  as for gradient descent.

# Convergence of exact coordinate descent

## Proposition (Warga (1963))

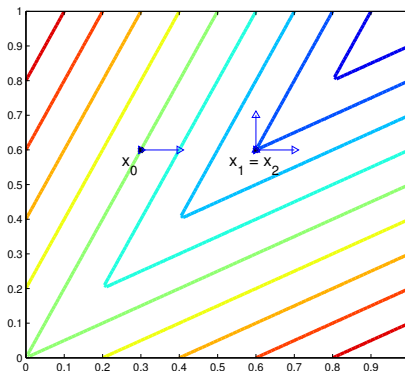
*Assume that*

- *$f$  is continuously differentiable*
- *$f$  is strictly convex*
- *there exists  $x_* \in \arg \min_{x \in X} f(x)$*

*then the exact coordinate descent method converges to  $x_*$ .*

# Counter-example: convex nonsmooth

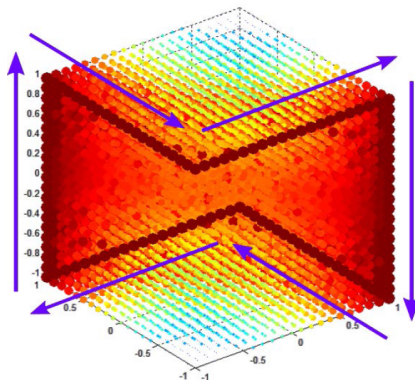
What if  $f$  is convex and non-smooth?



$$f(x^{(1)}, x^{(2)}) = |x^{(1)} - x^{(2)}| - \min(x^{(1)}, x^{(2)})$$

# Counter-example: smooth nonconvex

What is  $f$  is smooth and non-convex? (Example due to Powell)



$$f(x^{(1)}, x^{(2)}, x^{(3)}) = - (x^{(1)}x^{(2)} + x^{(2)}x^{(3)} + x^{(3)}x^{(1)}) + \sum_{i=1}^3 \max(0, |x^{(i)}| - 1)^2$$

# Adaboost

$y_j$  = label

$h_j$  = weak classifier

Minimise the exponential loss:

$$f(x) = \sum_{j=1}^m \exp(-y_j h_j^\top x).$$

Algorithm:

- Select the variable  $i_{k+1}$  such that  $i_{k+1} = \arg \max_i |\nabla_i f(x_k)|$  (greedy rule a.k.a. Gauss-Southwell rule, requires to compute the full gradient at each iteration)
- Perform exact coordinate descent along coordinate  $i_{k+1}$

If  $y_i \in \{-1, 1\}$  and  $h_j \in \{-1, 0, 1\}^n$ : closed form formulas

# Table of Contents

- 1 Exact coordinate descent
- 2 Coordinate gradient descent**
- 3 Proximal coordinate descent
- 4 Applications to ML estimators

# Motivation

- A 1D optimisation problem to solve at each iteration:  
This may be expensive
- We may solve it approximately since we've got plenty of iterations left
- We will do one single gradient step in the 1D problem



# Coordinate gradient descent

Parameters:  $\gamma_1, \dots, \gamma_n > 0$

Algorithm:

Choose  $i_{k+1} \in \{1, \dots, n\}$

$$\begin{cases} x_{k+1}^{(i)} = x_k^{(i)} - \gamma_i \nabla_i f(x_k) & \text{if } i = i_{k+1} \\ x_{k+1}^{(i)} = x_k^{(i)} & \text{if } i \neq i_{k+1} \end{cases}$$

# Coordinate gradient descent

Parameters:  $\gamma_1, \dots, \gamma_n > 0$

Algorithm:

Choose  $i_{k+1} \in \{1, \dots, n\}$

$$\begin{cases} x_{k+1}^{(i)} = x_k^{(i)} - \gamma_i \nabla_i f(x_k) & \text{if } i = i_{k+1} \\ x_{k+1}^{(i)} = x_k^{(i)} & \text{if } i \neq i_{k+1} \end{cases}$$

Choice of  $\gamma$ : coordinate-wise Lipschitz constant i.e. Lipschitz constant of

$$g_{i,x} : X_i \rightarrow \mathbb{R}$$

$$h \mapsto f(x + U_i h) = f(x^{(1)}, \dots, x^{(i-1)}, x^{(i)} + h, x^{(i+1)}, \dots, x^{(n)})$$

We will denote  $L_i = L(\nabla g_{i,x})$  this Lipschitz constant.

# Convergence speed

Assume  $f$  is convex;  $\nabla f$  is Lipschitz continuous;  $\forall i, \gamma_i = \frac{1}{L_i}$ .

## Proposition (Beck and Tetruashvili (2013))

If  $i_{k+1} = (k \bmod n) + 1$ , then

$$f(x_{k+1}) - f(x_*) \leq 4L_{\max}(1 + n^3 L_{\max}^2 / L_{\min}^2) \frac{R^2(x_0)}{k + 8/n}$$

where  $R^2(x_0) = \max_{x,y \in X} \{\|x - y\| : f(y) \leq f(x) \leq f(x_0)\}$ ,  
 $L_{\max} = \max_i L_i$  and  $L_{\min} = \min_i L_i$ .

**Note:**  $n^3$  can be prohibitive in high dimension. Due to pathological cases of the cyclic rule this bound is very very pessimistic (cf. linear regression).

# Convergence speed with randomization

Assume  $f$  is convex;  $\nabla f$  is Lipschitz continuous;  $\forall i, \gamma_i = \frac{1}{L_i}$ .

## Proposition (Nesterov (2012))

*If  $i_{k+1}$  is randomly generated, independently of  $i_1, \dots, i_k$  and  $\forall i \in \{1, \dots, n\}, \mathbb{P}(i_{k+1} = i) = \frac{1}{n}$ , then*

$$\mathbb{E}[f(x_{k+1}) - f(x_*)] \leq \frac{n}{k+n} \left( \left(1 - \frac{1}{n}\right)(f(x_0) - f(x_*)) + \frac{1}{2} \|x_* - x_0\|_L^2 \right)$$

*where  $\|x\|_L^2 = \sum_{i=1}^n L_i \|x^{(i)}\|_2^2$ .*

**Note:** As the algorithm is now stochastic the bounds are given in expectation.

# Comparison with gradient descent

The iteration complexity of the gradient descent method is

$$f(x_{k+1}) - f(x_*) \leq \frac{L(\nabla f)}{2(k+1)} \|x_* - x_0\|_2^2$$

To get an  $\epsilon$ -solution (*i.e.*, such that  $f(x_k) - f(x_*) \leq \epsilon$ ), we need at most  $\frac{L(\nabla f)}{2\epsilon} \|x_* - x_0\|_2^2$  iterations.

while for coordinate descent we need (omitting randomization)

$$\frac{n}{\epsilon} \left( \left(1 - \frac{1}{n}\right)(f(x_0) - f(x_*)) + \frac{1}{2} \|x_* - x_0\|_L^2 \right)$$

iterations.

# Comparison with gradient descent

How do the cost of iterations compare?

Let  $C$  the cost of one GD iteration and  $c$  the cost of one CD iteration.

Back to least square:  $C$  is the cost of computing  $\nabla f(x) = A^\top(Ax - b)$  which means  $C = O(\text{nnz}(A))$  or  $C = O(mn)$  for a dense matrix.

We have for CD,  $\nabla_i f(x) = U_i^\top A^\top(Ax - b)$  and with smart residual updates  $c = O(\text{nnz}(A))/n$  or  $C = O(m)$  for a dense matrix. So

$$c \approx C/n$$

# Comparison with gradient descent

Let's recall number of iterations for CD:

$$\frac{n}{\epsilon} \left( \left(1 - \frac{1}{n}\right)(f(x_0) - f(x_*)) + \frac{1}{2} \|x_* - x_0\|_L^2 \right)$$

- $f(x_0) - f(x_*) \leq \frac{L(\nabla f)}{2} \|x_0 - x_*\|_2^2$  and it may happen that  $f(x_0) - f(x_*) \ll \frac{L(\nabla f)}{2} \|x_0 - x_*\|_2^2$
- $L(\nabla f) = \lambda_{\max}(A^\top A)$  and  $L_i = a_i^\top a_i$  with  $a_i = AU_i$ . We always have  $L_i \leq L(\nabla f)$  and it may happen that  $L_i = O(L(\nabla f)/n)$ .
- So in the quadratic case,  $C_{CD} \leq C_{GD}$  and we may have  $C_{CD} = O(C_{GD}/n)$ .
- Explains the results in the notebook...

# Table of Contents

- 1 Exact coordinate descent
- 2 Coordinate gradient descent
- 3 Proximal coordinate descent**
- 4 Applications to ML estimators



# CD for composite separable problem?

Let us consider:

$$F(x) = f(x) + \sum_{i=1}^n g_i(x^{(i)}) ,$$

with

- $f$  convex, differentiable
- each  $g_i$  convex

The non-smooth part is here separable.

**Question:** Does

$$F(x + dU_i) \geq F(x) \quad \forall d \in \mathbb{R}, \quad \forall i \stackrel{?}{\Rightarrow} F(x) = \min_z F(z)$$

# CD for composite separable problem?

$$\begin{aligned} F(y) - F(x) &\geq \nabla f(x)^\top (y - x) + \sum_{i=1}^n (g_i(y^{(i)}) - g_i(x^{(i)})) \\ &\geq \sum_{i=1}^n \underbrace{\left[ \nabla_i f(x)(y^{(i)} - x^{(i)}) + (g_i(y^{(i)}) - g_i(x^{(i)})) \right]}_{\geq 0} \\ &\geq 0 \end{aligned}$$

This suggests that it should work ...

# Proximal coordinate descent

Parameters:  $\gamma_1, \dots, \gamma_n > 0$

Algorithm:

Choose  $i_{k+1} \in \{1, \dots, n\}$

$$\begin{cases} x_{k+1}^{(i)} = \text{prox}_{\gamma_i, g_i} \left( x_k^{(i)} - \gamma_i \nabla_i f(x_k) \right) & \text{if } i = i_{k+1} \\ x_{k+1}^{(i)} = x_k^{(i)} & \text{if } i \neq i_{k+1} \end{cases}$$

$$\text{prox}_{\gamma, g}(y) = \arg \min_{x \in \mathbb{R}^n} g(x) + \frac{1}{2} \|x - y\|_{\gamma^{-1}}^2$$

$$\text{prox}_{\gamma_i, g_i}(y) = \arg \min_{x \in \mathbb{R}} g_i(x) + \frac{1}{2\gamma_i} (x - y)^2$$

→ proximal operators for  $g(x) = \lambda|x|$ ,  $g(x) = \lambda\|x\|_2^2$  and  $g(x) = \mathbb{I}_{[0,1]}(x)$ .

# Convergence speed

We want to minimize  $F = f + g$ .

Assume  $f$  and  $g$  are convex;  $\nabla f$  is Lipschitz continuous;

$\forall i, \gamma_i = \frac{1}{L_i}$ .

## Proposition (Richtárik and Takáč (2014))

*If  $i_{k+1}$  is randomly generated, independently of  $i_1, \dots, i_k$  and*

*$\forall i \in \{1, \dots, n\}, \mathbb{P}(i_{k+1} = i) = \frac{1}{n}$ , then*

$$\mathbb{E}[F(x_{k+1}) - F(x_*)] \leq \frac{n}{k+n} \left( \left(1 - \frac{1}{n}\right)(F(x_0) - F(x_*)) + \frac{1}{2} \|x_* - x_0\|_L^2 \right)$$

**Note:** One obtain the same rate as for non-composite objectives.

→ cf. Proof in lecture notes.

# Table of Contents

- 1 Exact coordinate descent
- 2 Coordinate gradient descent
- 3 Proximal coordinate descent
- 4 Applications to ML estimators**

# Regression and classification under sparsity constraints

$$\min_{x \in \mathbb{R}^n} F(x) = \min_{x \in \mathbb{R}^n} f(x) + \sum_{i=1}^n g_i(x^{(i)})$$

- Lasso:  $f(x) = \frac{1}{2} \|y - Ax\|^2$  and  $g(x) = \|x\|_1 = \sum_i |x^{(i)}|$
- $\ell_1$  log. reg.:  $f(x) = \log(\exp(-y \odot Ax) + 1)$  and  $g(x) = \|x\|_1$  where  $\odot$  is the elementwise product (Hadamard product).
- Box-constrained regression  $f(x) = \frac{1}{2} \|y - Ax\|^2$  s.t.  $\|x\|_\infty \leq \kappa$
- Non-negative least squares (NNLS)  $f(x) = \frac{1}{2} \|y - Ax\|^2$  s.t.  $x^{(i)} \geq 0$

**Note:** Generally the regularizer is separable non-smooth and the data fit is smooth.

→ write full algorithm for NNLS and Lasso

# Multi-output regression under sparsity constraints

Multi-task Lasso (k tasks):

$$\min_{x \in \mathbb{R}^{n \times k}} F(x) = \min_{x \in \mathbb{R}^{n \times k}} \frac{1}{2} \|Y - Ax\|_{Fro}^2 + \sum_{i=1}^n \|x^{(i,\cdot)}\|_2$$

where  $x^{(i,\cdot)}$  is the  $i$ th row of matrix  $x$ .

**Note:** Here the  $g$  is still separable yet blocks of coordinates are updated at each iteration (it's block proximal coordinate descent). First convergence proof due to Tseng (2001).

# Support vector machines

Coordinate descent can be applied to the SVM in the dual. If the primal with  $(y_i \in \{-1, 1\})$  reads:

$$\min_{w \in \mathbb{R}^p, b \in \mathbb{R}} C \sum_{i=1}^n \max(0, 1 - y_i(z_i^\top w + b)) + \frac{1}{2} \|w\|_2^2$$

the classical dual of SVM for binary classification is given by:

$$\max_{\alpha \in \mathbb{R}^n} -\frac{1}{2} \alpha^\top Q \alpha + \mathbf{1}^\top \alpha \text{ s.t. } y^\top \alpha = 0 \text{ and } 0 \leq \alpha \leq C \mathbf{1}$$

with  $Q_{ij} = y_i y_j z_i^\top z_j$ .

**Note:** Here  $w$  is the normal to the separating hyperplane and  $b$  is the intercept.

→ Derive the dual from the primal writing the Lagrangian and KKT optimality conditions.



# Support vector machines with SMO

The dual reads:

$$\max_{\alpha \in \mathbb{R}^n} -\frac{1}{2} \alpha^T Q \alpha + \mathbf{1}^T \alpha \text{ s.t. } y^T \alpha = 0 \text{ and } 0 \leq \alpha \leq C \mathbf{1}$$

Sequential minimal optimization or SMO (Platt, 1998) is a blockwise coordinate descent in blocks of 2. Instead of cycling, it chooses the next block greedily.

**Note:** This does not meet separability assumptions for convergence we have just seen.

**Note:** This is what is implemented in Scikit-Learn SVC and SVR estimators that use internally the libsvm C++ library.

# Support vector machines with SDCA

If one does not fit an intercept  $b$  the primal reads:

$$\min_{w \in \mathbb{R}^p} C \sum_{i=1}^n \max(0, 1 - y_i z_i^\top w) + \frac{1}{2} \|w\|_2^2$$

and a dual formulation becomes:

$$\max_{\alpha \in \mathbb{R}^n} -\frac{1}{2} \alpha^\top Q \alpha + \mathbf{1}^\top \alpha - \mathbb{I}_{[0,C]^n}(\alpha).$$

Proximal coordinate ascent applies to this problem. When using the stochastic approach this algorithm is called Stochastic Dual Coordinate Ascent (SDCA).

**Note:** This is what is implemented in Scikit-Learn LinearSVC when using parameter `dual=True`. It uses internally the liblinear C++ library.

→ Write an implementation of SDCA.

# Support vector machines with SDCA

## Proposition (Shalev-Shwartz and Zhang (2013))

Let us define a primal point  $w_k = Z^\top \text{Diag}(y) \alpha_k$ , where  $(\alpha_k)_{k \geq 0}$  is generated by SDCA. The duality gap satisfies for all  $K \geq n$ ,

$$\mathbb{E} \left[ \frac{1}{K} \sum_{k=K}^{2K-1} P(w_k) - D(\alpha_k) \right] \leq$$

$$\frac{n}{K+n} \left( \left(1 - \frac{1}{n}\right) (D(\alpha_*) - D(\alpha_0)) + \frac{1}{2} \|\alpha_* - \alpha_0\|_L^2 \right) + \frac{n}{2K} C^2 \sum_{i=1}^n L_i$$

where  $\forall i, L_i = y_i^2 \|z_i\|^2$ .

→ cf. Proof in lecture notes.

# Graphical Lasso

Let  $A \in \mathbb{R}^{n \times p}$ , where rows are independent Gaussian observations drawn from  $N(0, \Sigma)$ ,

The graphical Lasso estimator (Banerjee et al., 2007, Friedman et al., 2007) reads:

$$\min_{\Theta \in \mathbb{R}^{p \times p}} -\log \det \Theta + \text{tr} S \Theta + \lambda \|\Theta\|_1$$

where  $\|\Theta\|_1 = \sum_{ij} |\Theta_{ij}|$ .

It provides an estimate of  $\Sigma^{-1}$  (precision matrix) when  $S = A^\top A/n$  is the empirical covariance.

# Graphical Lasso

Stationarity conditions:

$$-\Theta^{-1} + S + \lambda \Gamma = 0$$

where  $\Gamma_{ij} \in \partial|\Theta_{ij}|$ . Posing  $W = \Theta^{-1}$ . It is possible to do a coordinate descent on  $W$ . See Friedman et al. (2007).

**Note:** With  $\lambda = 0$  one recovers the maximum likelihood estimator.

**Note:** This is implemented the *GraphLasso* estimator in Scikit-Learn or in the *glasso* package in R.