

# ASTR8150/PHYS8150

## Optimization

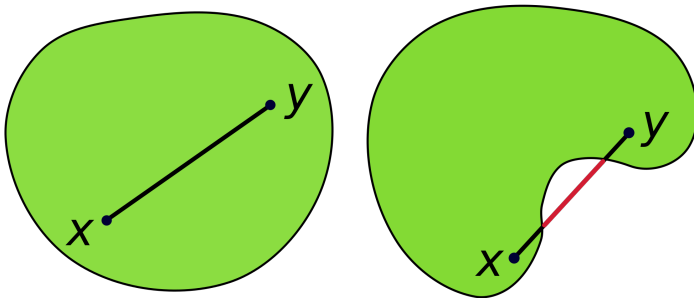
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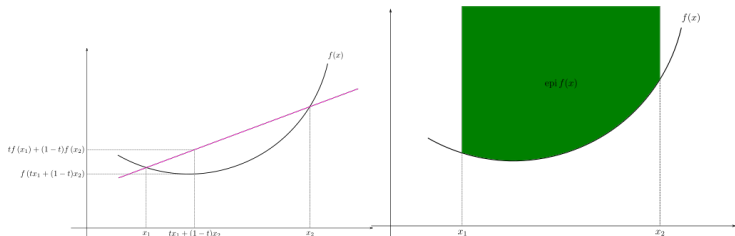
Fall 2023

# Convexity of a set



- In a convex set, for every pair of points within the region, every point on the straight line segment that joins the pair of points is also within the region.
- A set which is hollow or has an indent, for example, a crescent shape, is not convex.

# Convexity of a function



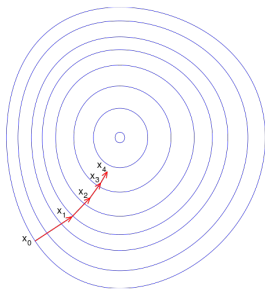
- A real-valued function is called convex if the set of points on or above the graph of the function (epigraph) is a convex set.
- For a twice differentiable function of a single variable, if the second derivative is always greater than or equal to zero for its entire domain then the function is convex. Examples:  $f(x) = x^2$  or  $f(x) = e^x$
- Jensen's inequality: if  $X$  is a convex set and  $f : X \rightarrow \mathbb{R}$ ,  $f$  is convex if:

$$\forall x_1, x_2 \in X, \forall t \in [0, 1] : \quad f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2).$$

# Smoothness of a function

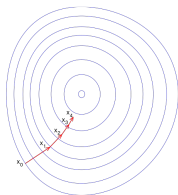
- The smoothness of a function is a property measured by the number of derivatives it has which are continuous. A smooth function is a function that has derivatives of all orders everywhere in its domain.
- The function  $f(x) = |x|^k$  is continuous and  $k$  times differentiable at all  $x$ . But at  $x = 0$  it is not  $(k + 1)$  times differentiable.
- The norms  $\ell_2$ ,  $\ell_1$  and pseudo-norm  $\ell_0$  are used in regularization.  $\ell_2$  is convex, differentiable and smooth.  $\ell_1$  is convex, differentiable but nonsmooth.  $\ell_0$  is non-convex and nonsmooth.

# Gradient descent (1)



- Gradient descent is based on the observation that if the multi-variable function  $f(\mathbf{x})$  is defined differentiable in a neighborhood of a point  $\mathbf{x}_0$ , then  $f(\mathbf{x})$  decreases "fastest" if one goes from  $\mathbf{x}_0$  in the direction of the negative gradient of  $f$  at  $\mathbf{x}_0$ ,  $-\nabla f(\mathbf{x}_0)$ .

## Gradient descent (2)



- It follows that, if

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha \nabla f(\mathbf{x}_n) \quad (1)$$

for  $\alpha$  small enough, then  $f(\mathbf{x}_n) \geq f(\mathbf{x}_{n+1})$ . In other words, the term  $\alpha \nabla f(\mathbf{x})$  is subtracted from  $\mathbf{x}$  because we want to move against the gradient, namely down toward the minimum.

- How can we choose  $\alpha$  ?
- The Rosenbrock function  $f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2$ . has a narrow curved valley which contains the minimum. The bottom of the valley is very flat. Because of the curved flat valley the optimization is zig-zagging slowly with small stepsizes towards the minimum.

# Steepest descent using line search

- **Inexact line search** consists in finding  $\alpha_k \simeq \underset{\alpha \in \mathbb{R}_+}{\operatorname{argmin}} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$
- The **line search** method is one of two basic iterative approaches to find a local minimum  $\mathbf{x}^*$  of an objective function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  using gradients. The other approach is **trust region**.

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## Algorithm 1 Steepest descent with line search

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1: procedure STEEPEST DESCENT( $f, \mathbf{x}$ )  
2:    $k = 0, \mathbf{x}_0$                                 ▷ Iteration counter + initial parameter guess  
3:   while  $\|\nabla f(\mathbf{x}_k)\| > \epsilon$  do                ▷  $\epsilon =$  tolerance  
4:      $\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$                         ▷ Descent direction = Steepest descent  
5:      $\alpha_k \simeq \underset{\alpha \in \mathbb{R}_+}{\operatorname{argmin}} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$     ▷ Line search  
6:      $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$   
7:      $k = k + 1$   
8:   end while  
9: end procedure
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# Nonlinear conjugate gradient methods

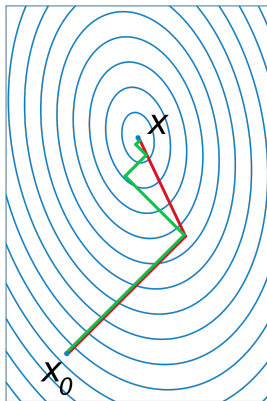
- Let's pose  $\mathbf{g}_k = \nabla f(x_k)$
- The steepest descent direction was  $\mathbf{d}_k = -\mathbf{g}_k$
- Conjugate directions differs from the steepest descent by attempting moves based on the history of the previous moves
- The descent direction for nonlinear conjugate gradient methods is

$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k, \quad \mathbf{d}_0 = -\mathbf{g}_0 \quad (2)$$

- The variation of the gradient is measured by  $\mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$
- The Conjugate Gradient update parameter  $\beta_k$  can be updated with different formulas



# Conjugate gradient: convergence



- A comparison of the linear convergence of simple gradient descent with optimal step size (in green) and the superlinear convergence of conjugate gradient (in red) for minimizing a quadratic function.

# Nonlinear conjugate gradient methods

$$\beta_k^{HS} = \frac{\mathbf{g}_{k+1}^\top \mathbf{y}_k}{\mathbf{d}_k^\top \mathbf{y}_k}$$

(1952) in the original (linear) CG paper  
of Hestenes and Stiefel [59]

$$\beta_k^{FR} = \frac{\|\mathbf{g}_{k+1}\|^2}{\|\mathbf{g}_k\|^2}$$

(1964) first nonlinear CG method, proposed  
by Fletcher and Reeves [45]

$$\beta_k^D = \frac{\mathbf{g}_{k+1}^\top \nabla^2 f(\mathbf{x}_k) \mathbf{d}_k}{\mathbf{d}_k^\top \nabla^2 f(\mathbf{x}_k) \mathbf{d}_k}$$

(1967) proposed by Daniel [39], requires  
evaluation of the Hessian  $\nabla^2 f(\mathbf{x})$

$$\beta_k^{PRP} = \frac{\mathbf{g}_{k+1}^\top \mathbf{y}_k}{\|\mathbf{g}_k\|^2}$$

(1969) proposed by Polak and Ribière [84]  
and by Polyak [85]

$$\beta_k^{CD} = \frac{\|\mathbf{g}_{k+1}\|^2}{-\mathbf{d}_k^\top \mathbf{g}_k}$$

(1987) proposed by Fletcher [44], CD  
stands for “Conjugate Descent”

$$\beta_k^{LS} = \frac{\mathbf{g}_{k+1}^\top \mathbf{y}_k}{-\mathbf{d}_k^\top \mathbf{g}_k}$$

(1991) proposed by Liu and Storey [67]

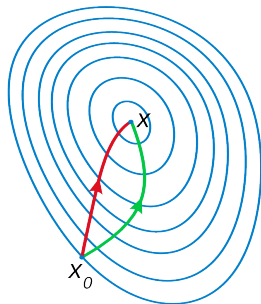
$$\beta_k^{DY} = \frac{\|\mathbf{g}_{k+1}\|^2}{\mathbf{d}_k^\top \mathbf{y}_k}$$

(1999) proposed by Dai and Yuan [27]

$$\beta_k^N = \left( \mathbf{y}_k - 2\mathbf{d}_k \frac{\|\mathbf{y}_k\|^2}{\mathbf{d}_k^\top \mathbf{y}_k} \right)^\top \frac{\mathbf{g}_{k+1}}{\mathbf{d}_k^\top \mathbf{y}_k}$$

(2005) proposed by Hager and Zhang [53]

# Newton optimization method



**Figure:** A comparison of gradient descent (green) and Newton's method (red) for minimizing a function (with small step sizes). Newton's method uses curvature information to take a more direct route.

- Hessian is used to exploit the curvature information

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha [\mathbf{H}f(\mathbf{x}_n)]^{-1} \nabla f(\mathbf{x}_n) \quad (3)$$

- $\alpha \in (0, 1)$ , with  $\alpha = 1$  the exact form.

# Newton-Raphson root-finding and eccentric anomaly

- Newton optimization method and Newton-Raphson's root finding methods are based on similar principles
- Newton-Raphson:  $x_{n+1} = x_n - f(x_n)/f'(x_n)$
- Example: the mean anomaly is proportional to time it is an easily measured quantity for an orbiting body. Given the mean anomaly  $M$ , find the eccentric anomaly  $E$  and the orbital eccentricity  $e$  with Kepler's Equation:

$$M = E - e \sin E \quad (4)$$

# Better than Newton: quasi-Newton methods

- Also known as variable metric methods, they avoid computing the Hessian then its inverse.
- The Broyden-Fletcher-Goldfarb-Shanno (BFGS) or Davidon-Fletcher-Powell (DFP) algorithms build iteratively approximations of  $[\mathbf{H}f(\mathbf{x}_n)]^{-1}$ .
- The most successful and well-known quasi-Newton method is the **Limited-memory BFGS (L-BFGS)** that approximates  $[\mathbf{H}f(\mathbf{x}_n)]^{-1}\nabla f(\mathbf{x}_n)$  directly and thus can work on large scale problems (millions of variables).
- New gradient descent variants attempt to deal with non-smooth functions (subgradient and bundle method).
- There are variants that deal with constrained minimization (i.e. bounds on variables or linearly tied variables) such as L-BFGS-B. Further refinements led to the VMLM algorithm in OptimPack.

# Trust-region method and Levenberg-Marquardt

- Consider the quadratic approximation of function  $f$  around  $x_0$ :

$$q(\epsilon) \simeq f(x_0) + \nabla f(x_0)\epsilon + \frac{1}{2}\epsilon^T \nabla^2 f(x_0)\epsilon \quad (5)$$

- $q(\epsilon)$  has a close-form minimum.
- $q(\epsilon)$  remains a good approximation within a given radius,  $\|e\|_2 < r^2$  defines the **trust region** radius  $r$ .
- The quadratic approximation predicts a certain reduction in the cost function,  $\Delta f_{\text{pred}}$ , which is compared to the true reduction  $\Delta f_{\text{actual}} = f(x) - f(x + \epsilon)$ . By looking at the ratio  $\Delta f_{\text{pred}}/\Delta f_{\text{actual}}$  we can estimate the trust-region size at each iteration, jump to the closed-form minimum within the trust region, and iterate.
- The **Levenberg-Marquardt** algorithm (first published in 1944 by Kenneth Levenberg, rediscovered in 1963 by Donald Marquardt) uses the trust-region approach with conjugate-gradients and Gauss-Newton (Newton optimized for non-linear  $\chi^2$ ). Like conjugate gradient and Newton, these local optimization.

# Derivative-free optimization methods

- **Derivative-free** optimization methods simply do not require gradient information
- Among the most popular local optimizer is **Nelder–Mead** method (aka downhill simplex method or amoeba method), which moves points of a polytope of  $n + 1$  vertices in  $n$ -parameter dimensions via reflection, contraction, expansion steps
- Most MCMC optimization methods.
- The NLOpt library provides mostly derivative-free algorithms, some of them for global optimization.

# Constrained minimization: the Lagrangian method

- **Constrained** minimization is minimization under equality or inequality constraints. **Bounded** optimization is a special case of constrained optimization where bounds are imposed on parameters (e.g. positivity, or variable within a range). In Bayesian terms, we're imposing a prior.
- A classic example is:

$$(\tilde{x}, \tilde{y}) = \underset{(x,y) \in \mathbb{R}^2}{\operatorname{argmin}} (x + y) \quad \text{s. t. } x^2 + y^2 = 1$$

- We pose  $g(x, y) = x^2 + y^2 - 1$  and the Lagrangian is:

$$\begin{aligned} \mathcal{L}(x, y, \lambda) &= f(x, y) + \lambda \cdot g(x, y) \\ &= x + y + \lambda(x^2 + y^2 - 1). \end{aligned}$$

where  $\lambda$  is a Lagrange multiplier.



# Constrained minimization: the Lagrangian method

- The gradient with respect to variables  $x, y$  and  $\lambda$

$$\begin{aligned}\nabla_{x,y,\lambda}\mathcal{L}(x,y,\lambda) &= \left(\frac{\partial\mathcal{L}}{\partial x}, \frac{\partial\mathcal{L}}{\partial y}, \frac{\partial\mathcal{L}}{\partial\lambda}\right) \\ &= (1 + 2\lambda x, 1 + 2\lambda y, x^2 + y^2 - 1)\end{aligned}$$

and therefore:

$$\nabla_{x,y,\lambda}\mathcal{L}(x,y,\lambda) = 0 \quad \Leftrightarrow \quad \begin{cases} 1 + 2\lambda x = 0 \\ 1 + 2\lambda y = 0 \\ x^2 + y^2 - 1 = 0 \end{cases}$$

- Solution  $x = y = -\frac{1}{2\lambda}$ ,  $\lambda \neq 0$ . Substituting into the last equation we get  $\lambda = \pm \frac{1}{\sqrt{2}}$  which implies that the stationary points of  $\mathcal{L}$  are  $\left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, -\frac{1}{\sqrt{2}}\right)$ ,  $\left(-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, \frac{1}{\sqrt{2}}\right)$ . And since  $f\left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right) = \sqrt{2}$  and  $f\left(-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right) = -\sqrt{2}$ , the solution is found.

# Constrained minimization: Half-quadratic splitting (1)

- Let's say we want to minimize:

$$\tilde{\mathbf{x}} = \underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \mu\Phi(\mathbf{x})$$

- If  $\Phi(\mathbf{x}) = \|\mathbf{W}\mathbf{x} - \mathbf{w}\|_2^2$ , Tikhonv gives us the solution  $\mathbf{x} = (\mathbf{H}^\top \mathbf{H} + \mathbf{W}^\top \mathbf{W})^{-1}(\mathbf{H}^\top \mathbf{y} + \mathbf{W}^\top \mathbf{w})$
- Other cases do not have closed-form solution, typical example is  $\Phi(\mathbf{x}) = \ell_1(\mathbf{x}) = \|\mathbf{x}\|_1$ .
- Splitting methods are methods that split the unconstrained problem into a constrained problem, using two different variables to represent the same one in different functions:

$$\begin{aligned} \tilde{\mathbf{x}} &= \underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \mu\Phi(\mathbf{z}) \quad \text{s.t.} \quad \mathbf{z} = \mathbf{x} \\ &= \underset{\mathbf{x}, \mathbf{z}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \mu\Phi(\mathbf{z}) + \frac{\rho}{2} \|\mathbf{z} - \mathbf{x}\|_2^2 \end{aligned}$$

# Constrained minimization: the two subproblems

- So we now want to minimize:

$$\mathcal{L}(\mathbf{x}, \mathbf{z}) = \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \mu\Phi(\mathbf{z}) + \frac{\rho}{2} \|\mathbf{z} - \mathbf{x}\|_2^2$$

- $\frac{\rho}{2} \|\mathbf{z} - \mathbf{x}\|_2^2$  is called an augmented term, and  $\rho$  is the augmented penalty hyperparameter.
- The **half-quadratic splitting method** solves iteratively (iteration variable =  $k$ ) the problem with respect to  $\mathbf{x}$ , then  $\mathbf{z}$ :

$$\tilde{\mathbf{x}}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \frac{\rho}{2} \|\tilde{\mathbf{z}}^k - \mathbf{x}\|_2^2 \quad \mathbf{x} \text{ sub-problem}$$

$$\tilde{\mathbf{z}}^{k+1} = \underset{\mathbf{z}}{\operatorname{argmin}} \frac{\rho}{2} \|\mathbf{z} - \tilde{\mathbf{x}}^{k+1}\|_2^2 + \mu\Phi(\mathbf{z}) \quad \mathbf{z} \text{ sub-problem}$$

and then increases  $\rho$  from initially low values to higher and higher ones.

# Constrained minimization: analytical solutions exist

- Why is this easier than the original problem ?

$$\tilde{\mathbf{x}}^{k+1} = \operatorname{argmin}_{\mathbf{x}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \frac{\rho}{2} \|\tilde{\mathbf{z}}^k - \mathbf{x}\|_2^2 \quad \mathbf{x} \text{ sub-problem}$$

$$\tilde{\mathbf{z}}^{k+1} = \operatorname{argmin}_{\mathbf{z}} \frac{\rho}{2} \|\mathbf{z} - \tilde{\mathbf{x}}^{k+1}\|_2^2 + \mu \Phi(\mathbf{z}) \quad \mathbf{z} \text{ sub-problem}$$

- The  $\mathbf{x}$  sub-problem can be solved by classic Tikhonov.
- The  $\mathbf{z}$  sub-problem can be solved analytically for some functions, for which we know the solution of the problem:

$$\operatorname{prox}_f(\mathbf{x}) = \operatorname{argmin}_{\mathbf{z}} \left( \frac{1}{2} \|\mathbf{z} - \mathbf{x}\|_2^2 + f(\mathbf{z}) \right)$$

- This solution  $\operatorname{prox}_f(\mathbf{x})$  is the **proximal operator** for the function  $f$ . At each point  $\mathbf{x}$  it finds a close-by local minimum of  $f$ . Note that Tikhonov is

# Proximal operator for the $\ell_1$ norm and positivity

- One can demonstrate that the proximal operator for  $\ell_1$  norm is:

$$\text{prox}_{\alpha\ell_1}(\mathbf{x}) = \underset{\mathbf{z}}{\operatorname{argmin}} \left( \frac{1}{2} \|\mathbf{z} - \mathbf{x}\|_2^2 + \alpha\ell_1(\mathbf{z}) \right) = \operatorname{sign}(\mathbf{x}) \cdot \max(|\mathbf{x}| - \alpha, 0)$$

where  $\cdot$  is the Hadamard product.

- The proximal operator for positivity is the projection onto the positive set:

$$\text{prox}_{I_{\mathbb{R}^+}}(\mathbf{x}) = \underset{\mathbf{z} \in \mathbb{R}^+}{\operatorname{argmin}} \left( \frac{1}{2} \|\mathbf{x} - \mathbf{z}\|_2^2 \right) = \max(\mathbf{x}, 0)$$

# Half-quadratic splitting: beyond the 1:1 change of variable

- Half-quadratic splitting only involves analytical steps: the  $\mathbf{x}$  sub-problem is solved via Tikhonov and the  $\mathbf{z}$  sub-problem via proximal operators (provided it is known). Generalizing beyond  $\mathbf{z} = \mathbf{x}$ , we can also have more complex linear constraints under the form  $\mathbf{Ax} + \mathbf{Bz} + \mathbf{c} = 0$ .
- How should we solve the total variation problem, i.e. minimize  $\frac{1}{2} \|\mathbf{Hx} - \mathbf{y}\|_2^2 + \mu \ell_1(\nabla \mathbf{x})$  ?
- We only know the proximal operator for  $\ell_1(\mathbf{z})$  and not for  $\ell_1(\nabla \mathbf{z})$ . So while we could pose  $\mathbf{z} = \mathbf{x}$ , we wouldn't know how to solve the  $\mathbf{z}$  sub-problem in closed form. However we can pose  $\mathbf{z} = \nabla \mathbf{x}$ , leading to:

$$\mathcal{L}(\mathbf{x}, \mathbf{z}) = \frac{1}{2} \|\mathbf{Hx} - \mathbf{y}\|_2^2 + \mu \ell_1(\mathbf{z}) + \frac{\rho}{2} \|\mathbf{z} - \nabla \mathbf{x}\|_2^2$$

# Total variation solved via Half-quadratic splitting

$$\mathcal{L}(\mathbf{x}, \mathbf{z}) = \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \mu \ell_1(\mathbf{z}) + \frac{\rho}{2} \|\mathbf{z} - \nabla \mathbf{x}\|_2^2$$

- The  $\mathbf{x}$  sub-problem has the closed form Tikhonov solution:

$$\tilde{\mathbf{x}}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2 + \frac{\rho}{2} \|\tilde{\mathbf{z}}^k - \nabla \mathbf{x}\|_2^2 \quad \mathbf{x} \text{ sub-problem}$$

$$\implies \mathbf{H}^\top (\mathbf{H}\mathbf{x} - \mathbf{y}) - \rho \nabla^\top (\tilde{\mathbf{z}}^k - \nabla \mathbf{x}) = 0$$

$$\implies \tilde{\mathbf{x}}^{k+1} = (\mathbf{H}^\top \mathbf{H} + \rho \nabla^\top \nabla)^{-1} (\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k)$$

- The  $\mathbf{z}$  sub-problem has a closed form proximal solution:

$$\tilde{\mathbf{z}}^{k+1} = \underset{\mathbf{z}}{\operatorname{argmin}} \mu \ell_1(\mathbf{z}) + \frac{\rho}{2} \|\mathbf{z} - \nabla \tilde{\mathbf{x}}^{k+1}\|_2^2 \quad \mathbf{z} \text{ sub-problem}$$

$$= \operatorname{prox}_{\frac{\mu}{\rho} \ell_1}(\nabla \tilde{\mathbf{x}}^{k+1}) = \operatorname{sign}(\nabla \tilde{\mathbf{x}}^{k+1}) \cdot \max(|\nabla \tilde{\mathbf{x}}^{k+1}| - \frac{\mu}{\rho}, 0)$$

# Making the $\mathbf{x}$ step faster: some tricks

- The  $\mathbf{x}$  sub-problem is the slowest one since it involves:

$$\tilde{\mathbf{x}}^{k+1} = (\mathbf{H}^\top \mathbf{H} + \rho \nabla^\top \nabla)^{-1} (\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k)$$

but matrix inversion is  $\sim \mathcal{O}(N^3)$  process for a  $N \times N$  matrix, and thus costly both in memory space and computing time. To work with larger images, tricks to speed up the inversion are used in practice.

- One is to use **sparse arrays** that only store the non-zero elements of  $\mathbf{H}$  and  $\nabla$ . The inversion and subsequent multiplication are then faster.
- Using an **orthogonal wavelet basis**,  $\mathbf{W}$ , as a sparsity basis instead of the spatial gradient  $\nabla$  since in this case  $\mathbf{W}^\top \mathbf{W} = \alpha \mathbf{I}$ .
- Another is to employ the backslash operator in Julia (or Matlab). We have  $\mathbf{X}^{-1} \mathbf{Y} = \mathbf{X} \backslash \mathbf{Y}$ , but the latter operation doesn't store the inverted matrix  $\mathbf{X}^{-1}$ ; instead it just temporarily stores the parts useful for its multiplication by  $\mathbf{Y}$ .

$$\tilde{\mathbf{x}}^{k+1} = (\mathbf{H}^\top \mathbf{H} + \rho \nabla^\top \nabla) \backslash (\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k)$$



# Making the x step faster: circulant matrices (1)

- It turns out  $\nabla^\top \nabla$  and  $\mathbf{H}^\top \mathbf{H}$  can be simplified if  $\nabla$  and  $\mathbf{H}$  are circulant matrices, or concatenation of circulant matrices. This is the case when  $\nabla$  is the spatial gradient, and when  $\mathbf{H}$  is a convolution (= if modeling the imaging done by an optical system).
- A circulant matrix  $\mathbf{C}$  takes the form:

$$\mathbf{C} = \begin{bmatrix} c_1 & c_n & \dots & c_3 & c_2 \\ c_2 & c_1 & c_n & & c_3 \\ \vdots & c_2 & c_1 & \ddots & \vdots \\ c_{n-1} & \vdots & \ddots & \ddots & c_n \\ c_n & c_{n-1} & \dots & c_2 & c_1 \end{bmatrix}.$$

- All circulant matrixes can be written as  $\mathbf{C} = \mathbf{F} \mathbf{D} \mathbf{F}^\top$  where  $\mathbf{F}$  is the Fourier transform ( $n^2 \times n^2$  if implemented via matrix operations) and  $\mathbf{D} = \text{diag}(\mathbf{F}([c_1 \dots c_n]))$  is diagonal.

# Making the x step faster: circulant matrices (2)

- We remind that  $\mathbf{F}^\top \mathbf{F} = \mathbf{I}$  since  $\mathbf{F}^\top = \mathbf{F}^{-1}$  and  $(\mathbf{AB})^\top = \mathbf{B}^\top \mathbf{A}^\top$
- Since  $\mathbf{C} = \mathbf{FDF}^\top$ ,  $\mathbf{C}^\top = ((\mathbf{FD})\mathbf{F}^\top)^\top = \mathbf{F}(\mathbf{FD})^\top = \mathbf{FD}^\top \mathbf{F}^\top$
- Consequently  $\mathbf{C}^\top \mathbf{C} = \mathbf{FDF}^\top \mathbf{FD}^\top \mathbf{F}^\top = \mathbf{FD}^2 \mathbf{F}^\top$  since  $\mathbf{D}$  is diagonal.
- The application relies on the fact that applying the Fourier transforms  $\mathbf{F}$  or  $\mathbf{F}^{-1}$  can be done with very fast FFT algorithms:

$$\begin{aligned}(\mathbf{H}^\top \mathbf{H} + \rho \nabla^\top \nabla) \tilde{\mathbf{x}}^{k+1} &= \mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k \\(\mathbf{FDH}^2 \mathbf{F}^\top + \rho \mathbf{FD} \nabla^2 \mathbf{F}^\top) \tilde{\mathbf{x}}^{k+1} &= \mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k \\ \mathbf{F}(\mathbf{D}_H^2 + \rho \mathbf{D}_\nabla^2) \mathbf{F}^\top \tilde{\mathbf{x}}^{k+1} &= \mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k \\ (\mathbf{D}_H^2 + \rho \mathbf{D}_\nabla^2) \mathbf{F}^\top \tilde{\mathbf{x}}^{k+1} &= \mathbf{F}^{-1}(\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k) \\ \mathbf{F}^\top \tilde{\mathbf{x}}^{k+1} &= \frac{\mathbf{F}^{-1}(\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k)}{\mathbf{D}_H^2 + \rho \mathbf{D}_\nabla^2} \\ \tilde{\mathbf{x}}^{k+1} &= \mathbf{F} \left( \frac{\mathbf{F}^{-1}(\mathbf{H}^\top \mathbf{y} + \rho \nabla^\top \tilde{\mathbf{z}}^k)}{\mathbf{D}_H^2 + \rho \mathbf{D}_\nabla^2} \right)\end{aligned}$$

# Augmented Lagrangian methods

- Let's say we want to minimize  $f(\mathbf{x})$  under a sets of constraints on  $\mathbf{x}$ . We saw we could express each of these constrains as  $g_i(\mathbf{x}) = 0$ . Then we just need to minimize the Lagrangian:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_i \lambda_i \cdot g_i(\mathbf{x})$$

where  $\boldsymbol{\lambda}$  is a vector this time.

- The idea is to use an **augmented Lagrangian**:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_i \lambda_i \cdot g_i(\mathbf{x}) + \frac{\rho}{2} \sum_i |g_i(\mathbf{x})|^2$$

where the augmentation term  $\sum_i |g_i(\mathbf{x})|^2$  is multiplied by penalty terms  $\rho$ .

- The **method of multipliers** solves this by iterating:

$$\mathbf{x}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} \mathcal{L}(\mathbf{x}, \lambda_i^k)$$

$$\lambda_i^{k+1} = \lambda_i^k + \rho^k g_i(\mathbf{x}^k) \quad \forall i$$

## Example: Method of multipliers for linear constraints

- Let's say we want to minimize  $f(\mathbf{x})$  under a sets of linear constraints on  $\mathbf{x}$ , we can express them as  $\mathbf{Ax} = \mathbf{b}$ .
- The augmented Lagrangian is:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}^\top (\mathbf{Ax} - \mathbf{b}) + \frac{\rho}{2} \|\mathbf{Ax} - \mathbf{b}\|_2^2$$

- The method of multipliers solves this by iterating:

$$\mathbf{x}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^k)$$

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \rho(\mathbf{Ax}^{k+1} - \mathbf{b})$$

# Alternating Direction Method of Multipliers (ADMM)

- Putting all our previous knowledge together, using variable splitting, Lagrangian multipliers, and augmentation terms, we come with ADMM, a method to solve:

$$\underset{\mathbf{x}, \mathbf{z}}{\operatorname{argmin}} f(\mathbf{x}) + g(\mathbf{z}) \quad \text{s.t. } \mathbf{Ax} + \mathbf{Bz} + \mathbf{c} = \mathbf{0}$$

- ADMM solves this by posing:

$$\mathcal{L}(\mathbf{x}, \mathbf{z}, \boldsymbol{\lambda}) = f(\mathbf{x}) + g(\mathbf{z}) + \boldsymbol{\lambda}^\top (\mathbf{Ax} + \mathbf{Bz} + \mathbf{c}) + \frac{\rho}{2} \|\mathbf{Ax} + \mathbf{Bz} + \mathbf{c}\|_2^2$$

- And then we iterate:

$$\begin{aligned}\mathbf{x}^{k+1} &= \underset{\mathbf{x}}{\operatorname{argmin}} \mathcal{L}(\mathbf{x}, \mathbf{z}^k, \boldsymbol{\lambda}^k) = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x}) + \frac{\rho}{2} \left\| \mathbf{Ax} + \mathbf{Bz}^k + \mathbf{c} + \frac{\boldsymbol{\lambda}^k}{\rho} \right\|_2^2 \\ \mathbf{z}^{k+1} &= \underset{\mathbf{z}}{\operatorname{argmin}} \mathcal{L}(\mathbf{x}^{k+1}, \mathbf{z}, \boldsymbol{\lambda}^k) = \underset{\mathbf{z}}{\operatorname{argmin}} g(\mathbf{z}) + \frac{\rho}{2} \left\| \mathbf{Ax}^{k+1} + \mathbf{Bz} + \mathbf{c} + \frac{\boldsymbol{\lambda}^k}{\rho} \right\|_2^2 \\ \boldsymbol{\lambda}^{k+1} &= \boldsymbol{\lambda}^k + \rho(\mathbf{Ax}^{k+1} + \mathbf{Bz}^{k+1} + \mathbf{c})\end{aligned}$$

- For convenience we often find in paper the scaled form of ADMM, using the lagragian multiplier  $\eta = \lambda/\rho$

$$\mathbf{x}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x}) + \frac{\rho}{2} \left\| \mathbf{Ax} + \mathbf{Bz}^k + \mathbf{c} + \boldsymbol{\eta}^k \right\|_2^2$$

$$\mathbf{z}^{k+1} = \underset{\mathbf{z}}{\operatorname{argmin}} g(\mathbf{z}) + \frac{\rho}{2} \left\| \mathbf{Ax}^{k+1} + \mathbf{Bz} + \mathbf{c} + \boldsymbol{\eta}^k \right\|_2^2$$

$$\boldsymbol{\eta}^{k+1} = \boldsymbol{\eta}^k + (\mathbf{Ax}^{k+1} + \mathbf{Bz}^{k+1} + \mathbf{c})$$

- $\boldsymbol{\eta}$  is just the running sum of residuals.

# ADMM residuals and convergence

- Primal residual:  $\mathbf{r}^{k+1} = \mathbf{A}\mathbf{x}^{k+1} + \mathbf{B}\mathbf{z}^{k+1} + \mathbf{c}$ , i.e. checks if the relation between  $\mathbf{x}$  and  $\mathbf{z}$  works.
- Dual residual:  $\mathbf{s} = \rho \mathbf{A}^\top \mathbf{B}(\mathbf{z}^{k+1} - \mathbf{z}^k)$ , i.e. if  $\mathbf{z}$  has converged
- Convergence properties: global convergence of the iterative procedure to a local optimum is guaranteed. Slow (linear) rate of convergence, slower than gradient-based methods in theory. But the steps can be made very fast.
- Adaptive ADMM modifies  $\rho$  based on heuristics such as residual norm balancing or spectral methods.

# ADMM: application to TV regularization with Gaussian likelihood

- Like with half quadratic, we pose  $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{H}\mathbf{x} - \mathbf{y}\|_2^2$ ,  $g(\mathbf{z}) = \ell_1(\mathbf{z})$  and  $\mathbf{z} = \nabla \mathbf{x}$ , i.e.  $\mathbf{A} = \nabla$ ,  $\mathbf{B} = -\mathbf{I}$  and  $\mathbf{c} = \mathbf{0}$ .

$$\mathbf{x}^{k+1} = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x}) + \frac{\rho}{2} \left\| \nabla \mathbf{x} - \mathbf{z}^k + \boldsymbol{\eta}^k \right\|_2^2 \rightarrow \text{Tikhonov}$$

$$\mathbf{z}^{k+1} = \underset{\mathbf{z}}{\operatorname{argmin}} g(\mathbf{z}) + \frac{\rho}{2} \left\| \nabla \mathbf{x}^{k+1} - \mathbf{z} + \boldsymbol{\eta}^k \right\|_2^2 \rightarrow \text{Proximal operator for } g$$

$$\boldsymbol{\eta}^{k+1} = \boldsymbol{\eta}^k + \nabla \mathbf{x}^{k+1} - \mathbf{z}^{k+1}$$

These steps are very similar to Half Quadratic, with just the addition of  $\boldsymbol{\eta}$  in the squared norms.



# Consensus ADMM

- Consensus ADMM is solving  $\operatorname{argmin}_{\mathbf{x}} \sum_{i=1}^N f_i(\mathbf{x})$  by recasting it as:

$$\operatorname{argmin}_{\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{x}} \sum_{i=1}^N f_i(\mathbf{x}_i) \quad \text{s.t. } \mathbf{x}_i = \mathbf{x}, \quad \forall i.$$

- Used to add more regularization terms. But more importantly if the log-likelihood can be split (into different wavelengths, epochs, etc.), such as is often the case with  $\chi^2$  then ADMM allows for **efficient parallelization** of large-scale problems.
- Reminder:  $k$  = iteration index,  $i$  = term index.

$$\mathbf{x}_i^{k+1} = \operatorname{argmin}_{\mathbf{x}_i} f_i(\mathbf{x}_i) + \frac{\rho}{2} \left\| \mathbf{x}_i - \mathbf{x}^k + \boldsymbol{\eta}^k \right\|_2^2 \rightarrow \text{computed in parallel}$$

$$\mathbf{x}^{k+1} = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_i^{k+1} + \boldsymbol{\eta}^k) \rightarrow \text{consensus step, fast}$$

$$\boldsymbol{\eta}^{k+1} = \boldsymbol{\eta}^k + \mathbf{x}_i^{k+1} - \mathbf{x}^{k+1} \rightarrow \text{fast}$$

# Interesting ADMM papers

- Deblurring with Poisson noise:  
<https://ieeexplore.ieee.org/document/5492199>
- Deblurring with unknown boundaries:  
<https://ieeexplore.ieee.org/document/6738120>